

# **Data Mining**

## **Classification: Basic Concepts, Decision Trees, and Model Evaluation**

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Lecture Notes for Chapter 4

Introduction to Data Mining  
by  
Tan, Steinbach, Kumar

# Classification: Definition

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- Given a collection of records (*training set*)
  - Each record contains a set of *attributes*, one of the attributes is the *class*.
- Find a *model* for class attribute as a function of the values of other attributes.
- Goal: previously unseen records should be assigned a class as accurately as possible.
  - A *test set* is used to determine the accuracy of the model. Usually, the given data set is divided into training and test sets, with training set used to build the model and test set used to validate it.

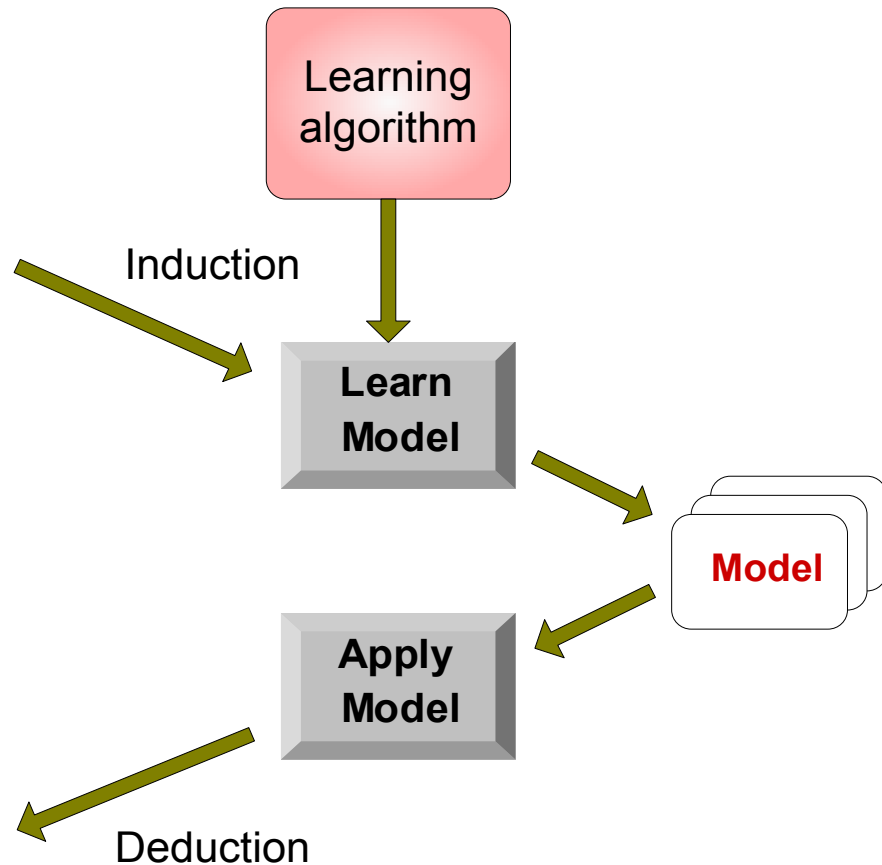
# Illustrating Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set

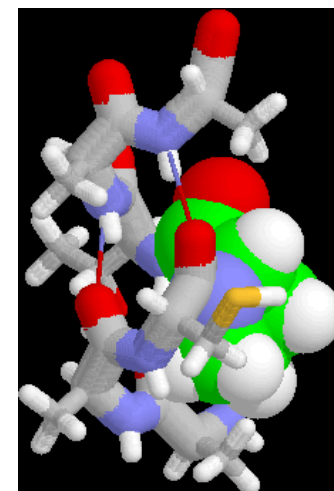
Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set



# Examples of Classification Task

- Predicting tumor cells as benign or malignant
- Classifying credit card transactions as legitimate or fraudulent
- Classifying secondary structures of protein as alpha-helix, beta-sheet, or random coil
- Categorizing news stories as finance, weather, entertainment, sports, etc



# Classification Techniques

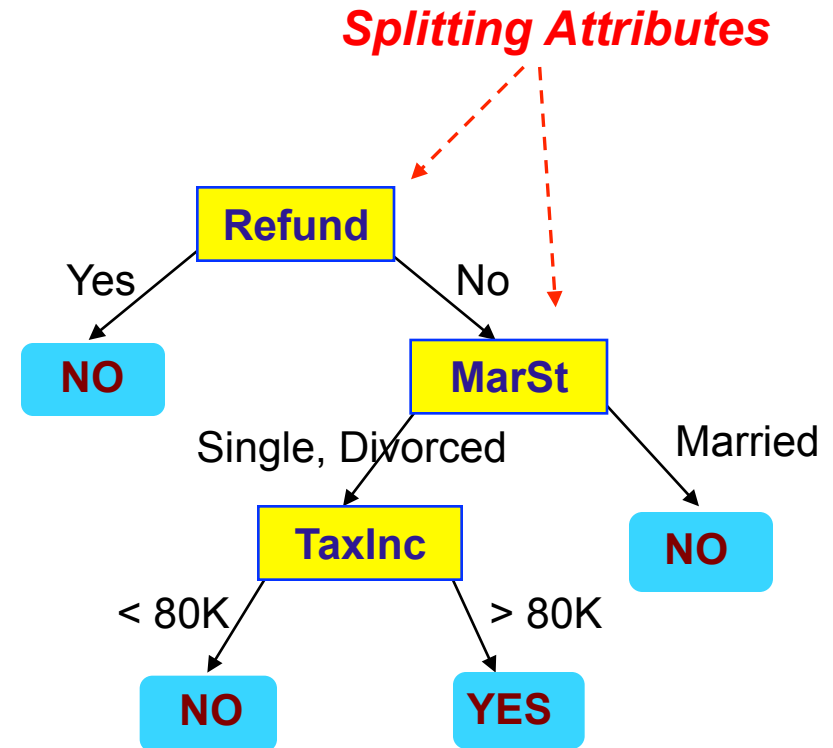
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- Decision Tree based Methods
- Rule-based Methods
- Memory based reasoning
- Neural Networks
- Naïve Bayes and Bayesian Belief Networks
- Support Vector Machines

# Example of a Decision Tree

<i>Tid</i>	<i>Refund</i>	<i>Marital Status</i>	<i>Taxable Income</i>	<i>Cheat</i>
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

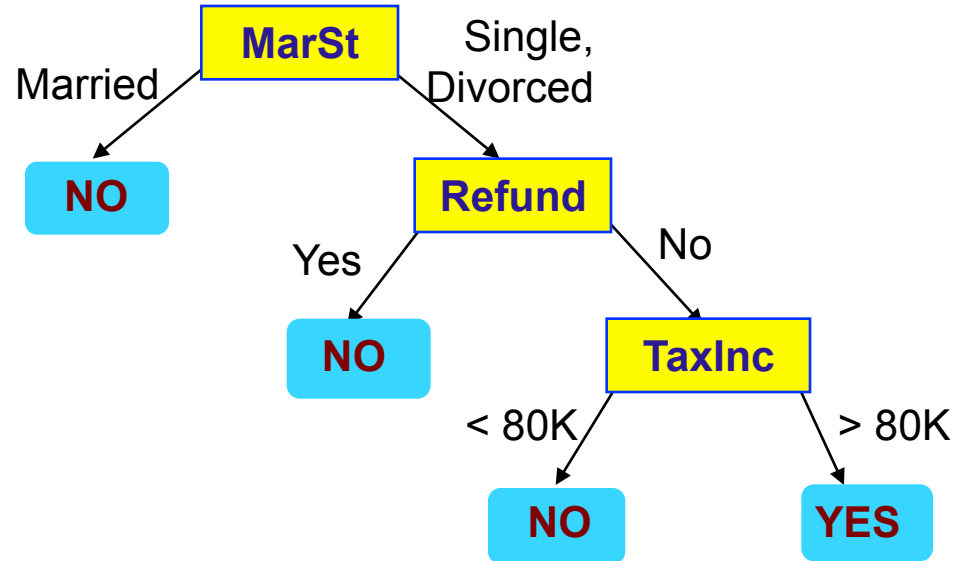
Training Data



Model: Decision Tree

# Another Example of Decision Tree

<i>Tid</i>	<i>Refund</i>	<i>Marital Status</i>	<i>Taxable Income</i>	<i>Cheat</i>
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



There could be more than one tree that fits the same data!

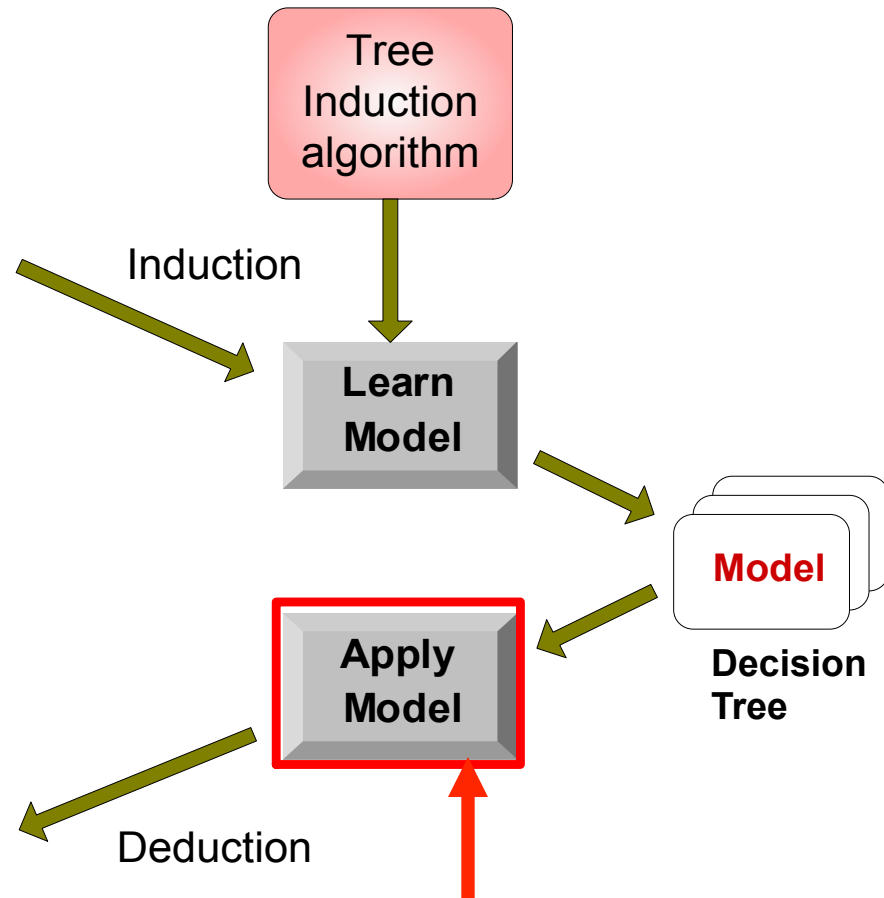
# Decision Tree Classification Task

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Training Set

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15	No	Large	67K	?

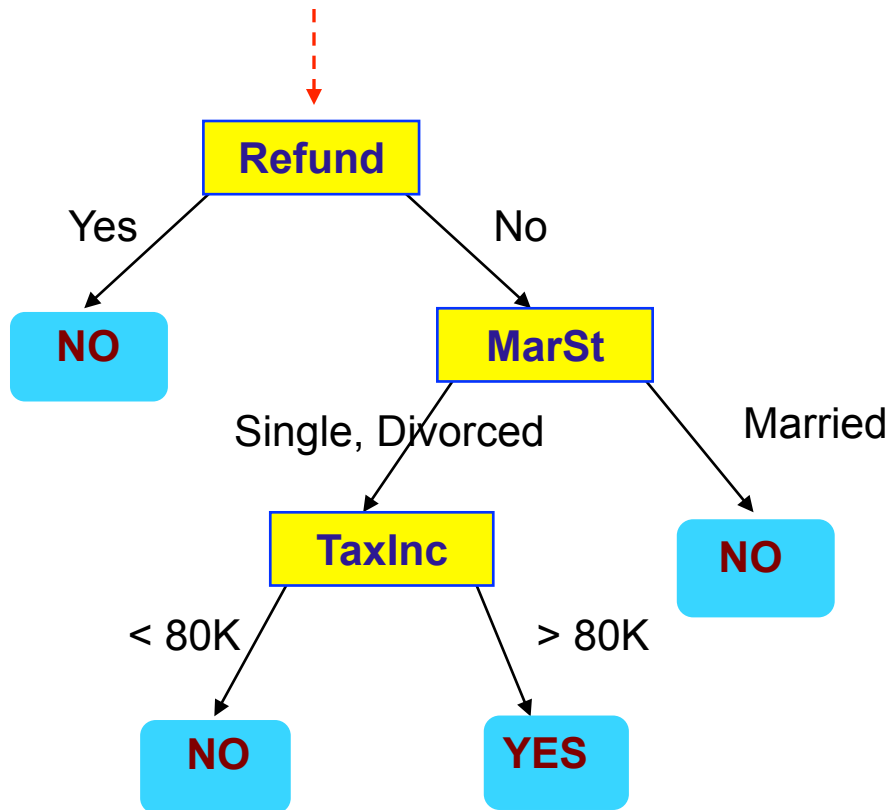
Test Set





# Apply Model to Test Data

Start from the root of tree.



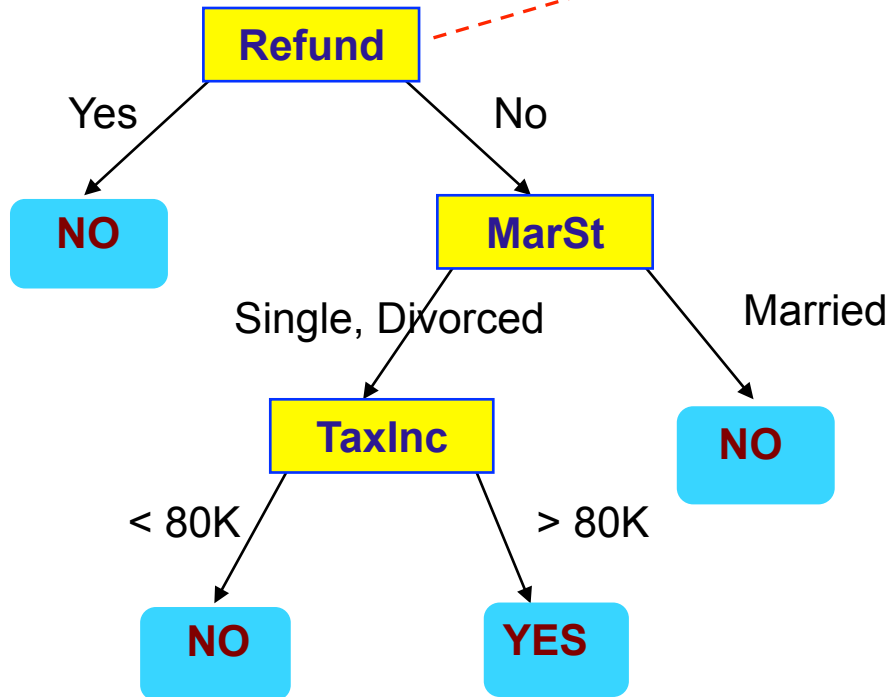
## Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

# Apply Model to Test Data

## Test Data

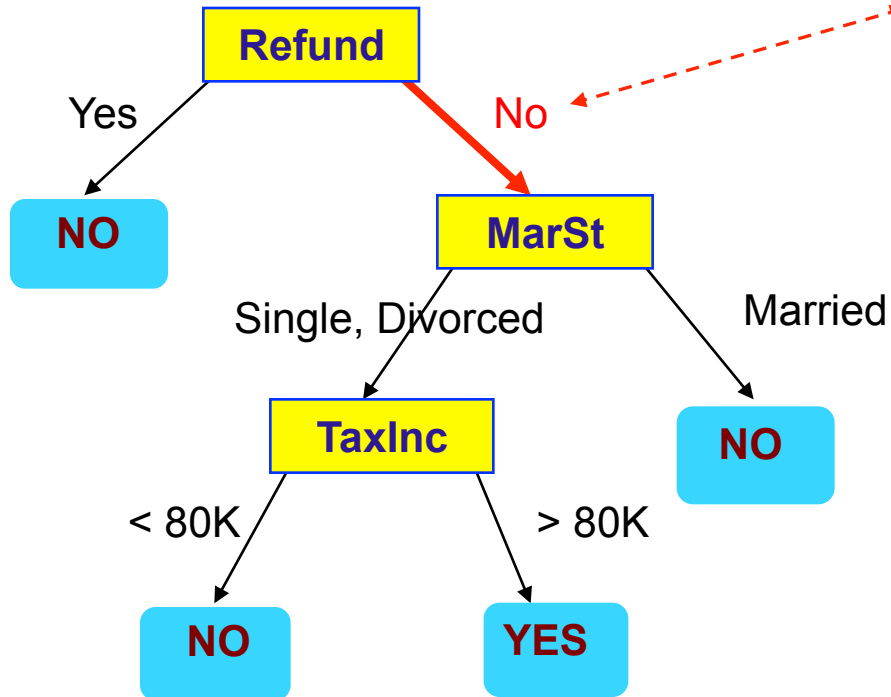
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



# Apply Model to Test Data

## Test Data

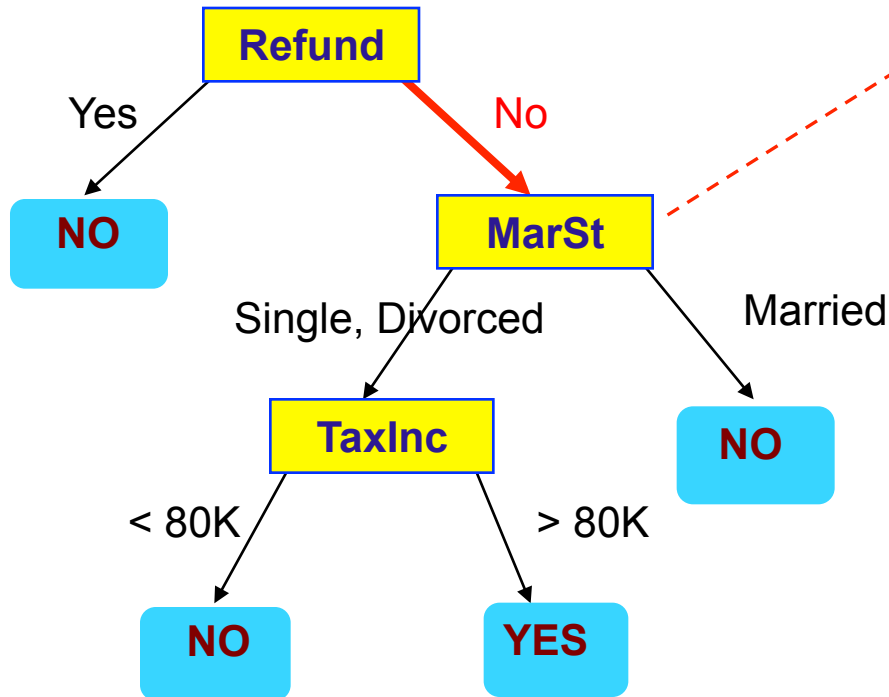
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



# Apply Model to Test Data

## Test Data

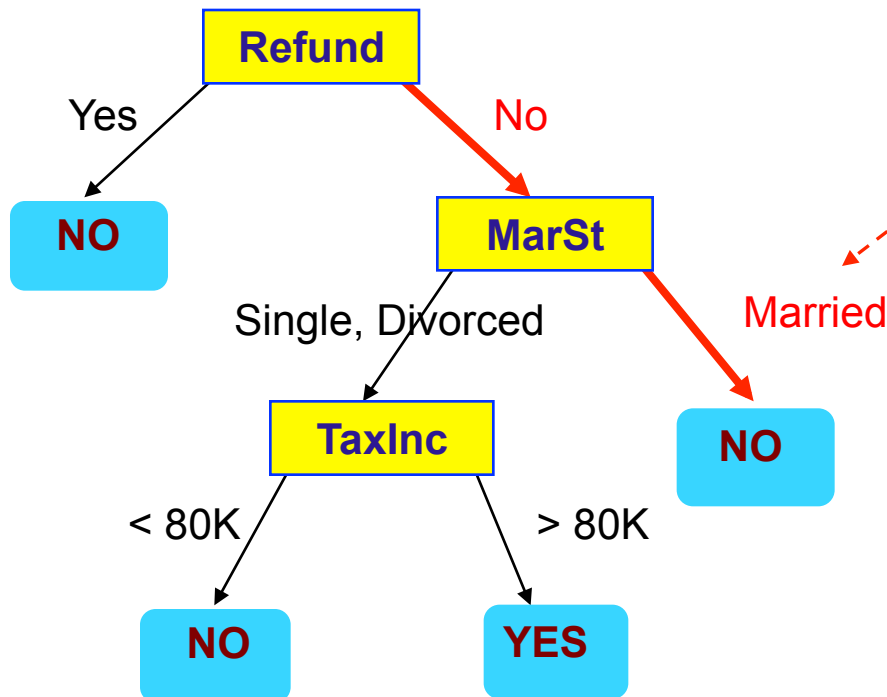
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



# Apply Model to Test Data

## Test Data

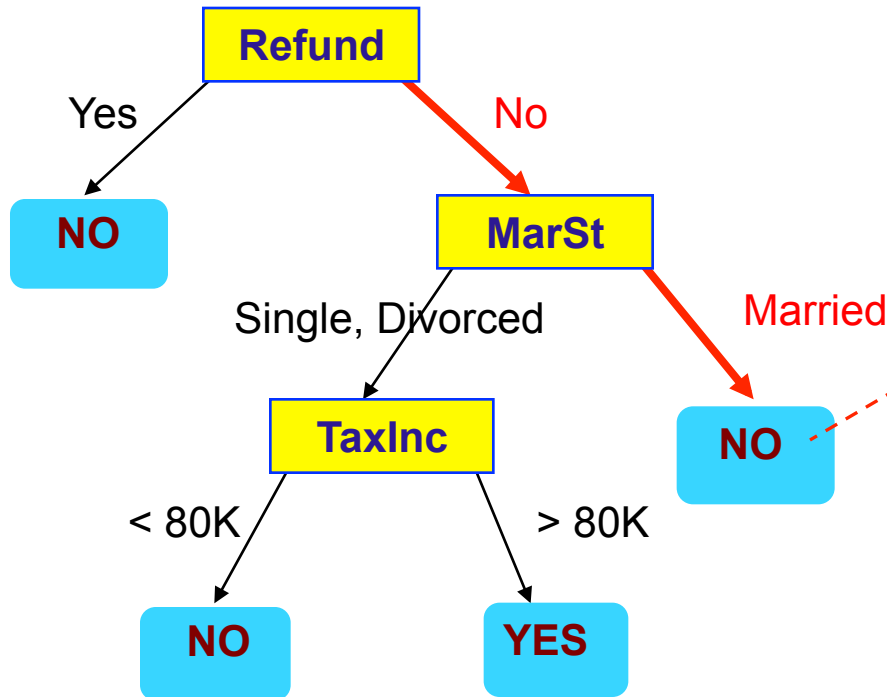
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



# Apply Model to Test Data

## Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Assign Cheat to "No"

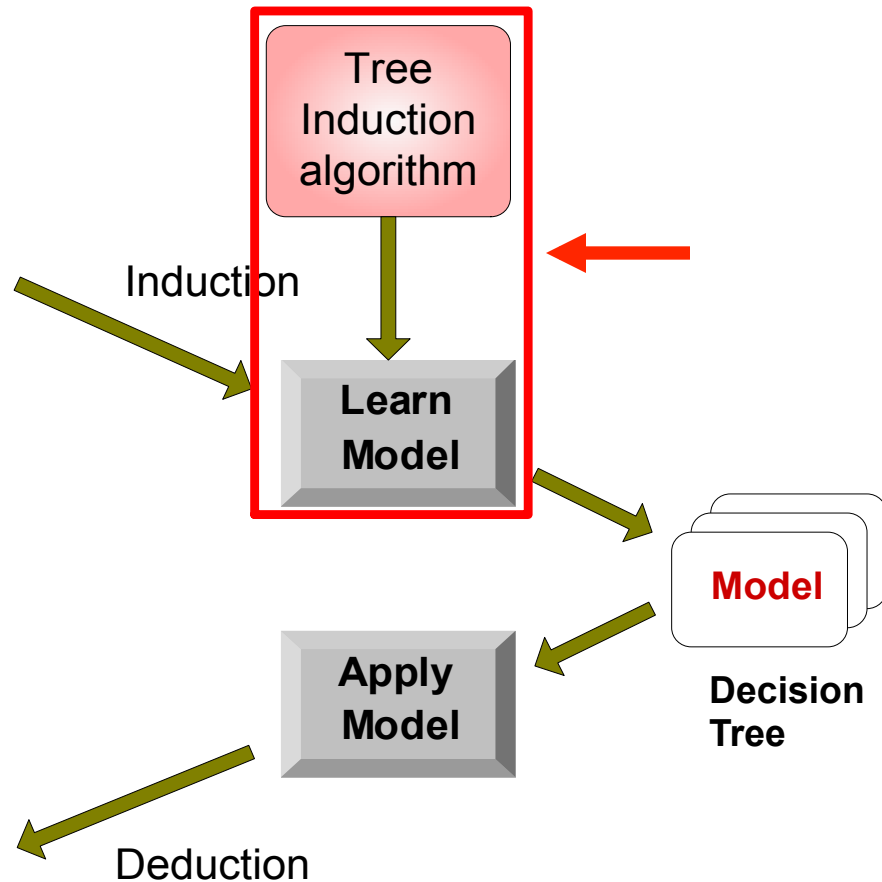
# Decision Tree Classification Task

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Training Set

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Test Set



# Decision Tree Induction

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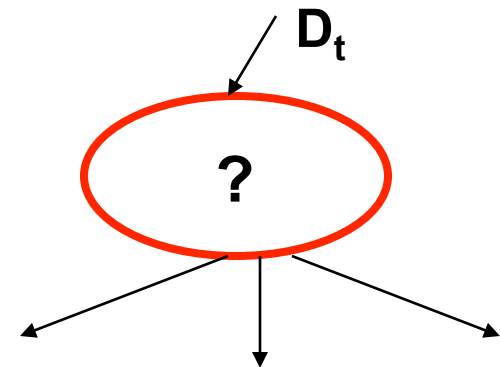
- Many Algorithms:
  - Hunt's Algorithm (one of the earliest)
  - CART
  - ID3, C4.5
  - SLIQ, SPRINT



# General Structure of Hunt's Algorithm

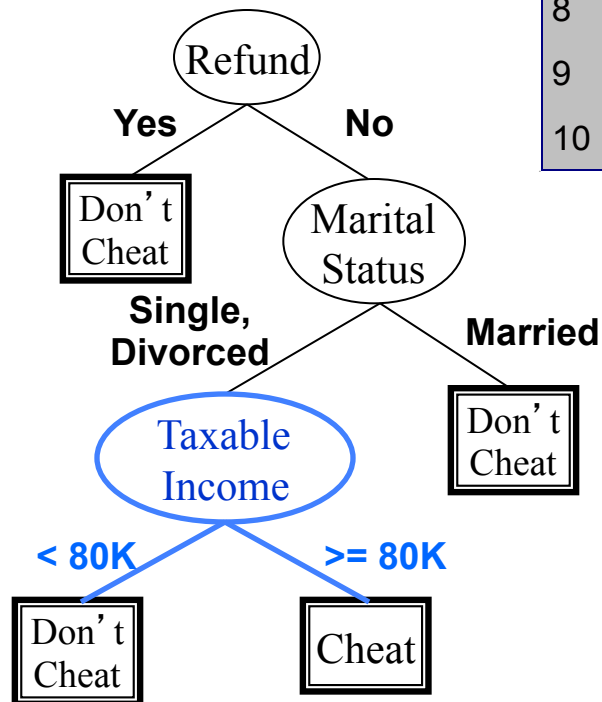
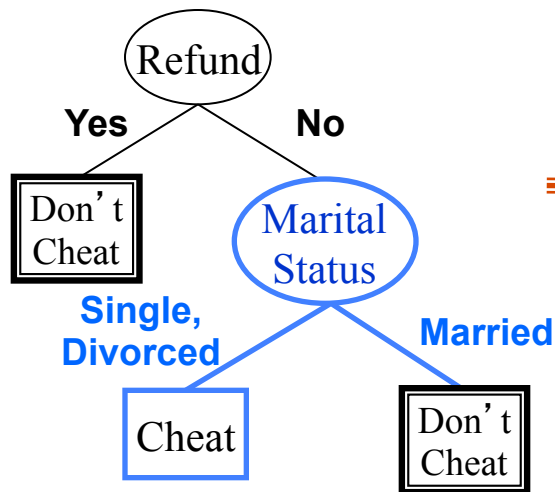
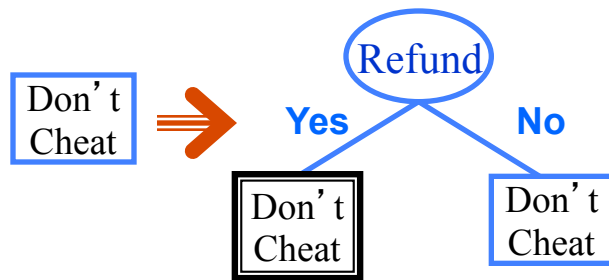
- Let  $D_t$  be the set of training records that reach a node  $t$
- General Procedure:
  - If  $D_t$  contains records that belong the same class  $y_t$ , then  $t$  is a leaf node labeled as  $y_t$
  - If  $D_t$  is an empty set, then  $t$  is a leaf node labeled by the default class,  $y_d$
  - If  $D_t$  contains records that belong to more than one class, use an attribute test to split the data into smaller subsets. Recursively apply the procedure to each subset.

<i>Tid</i>	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



# Hunt's Algorithm

Tid	Refund	Marital Status	Taxable Income	Cheat
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8	No	Single	85K	Yes
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10	No	Single	90K	Yes



# Tree Induction

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- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - ◆ How to specify the attribute test condition?
    - ◆ How to determine the best split?
  - Determine when to stop splitting

# Tree Induction

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- Greedy strategy.
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    - ◆ How to determine the best split?
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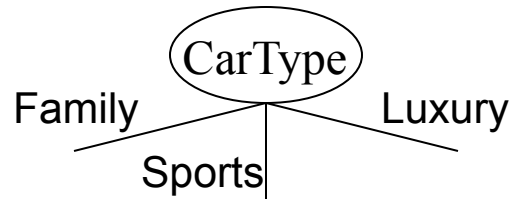
# How to Specify Test Condition?

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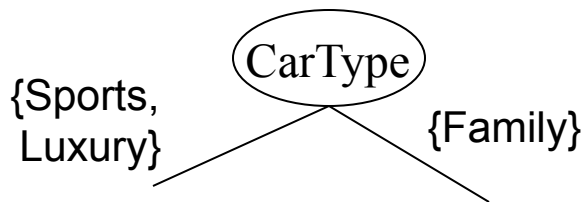
- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

# Splitting Based on **Nominal** Attributes

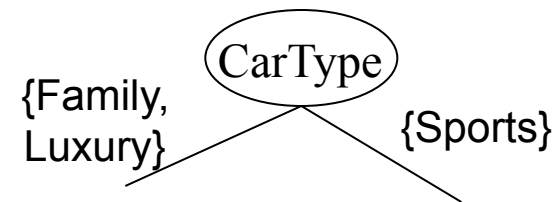
- **Multi-way split:** Use as many partitions as distinct values.



- **Binary split:** Divides values into two subsets.  
Need to find optimal partitioning.

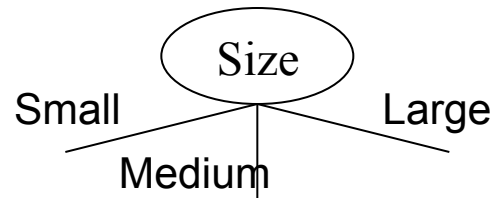


OR

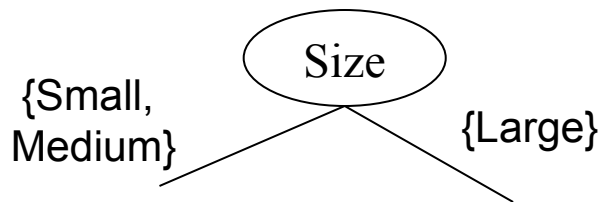


# Splitting Based on Ordinal Attributes

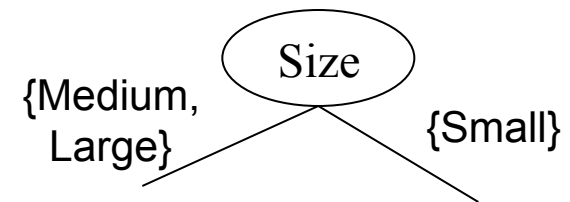
- **Multi-way split:** Use as many partitions as distinct values.



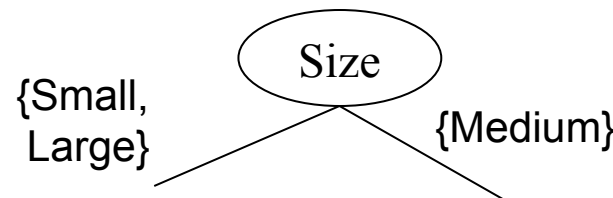
- **Binary split:** Divides values into two subsets.  
Need to find optimal partitioning.



OR



- **What about this split?**



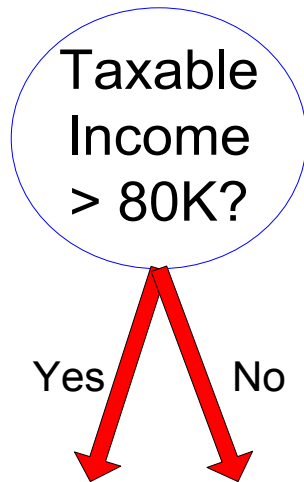
# Splitting Based on Continuous Attributes

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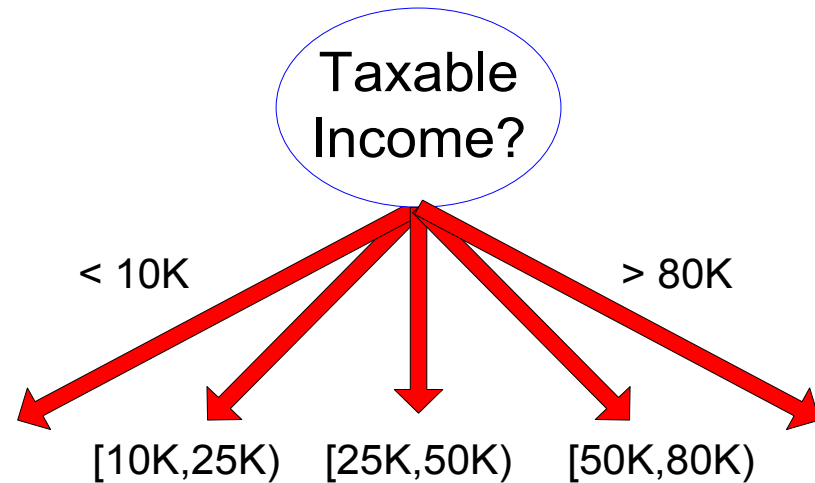
- Different ways of handling
  - **Discretization** to form an ordinal categorical attribute
    - ◆ Static – discretize once at the beginning
    - ◆ Dynamic – ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.
  - **Binary Decision**:  $(A < v)$  or  $(A \geq v)$ 
    - ◆ consider all possible splits and finds the best cut
    - ◆ can be more compute intensive



# Splitting Based on Continuous Attributes



(i) Binary split



(ii) Multi-way split

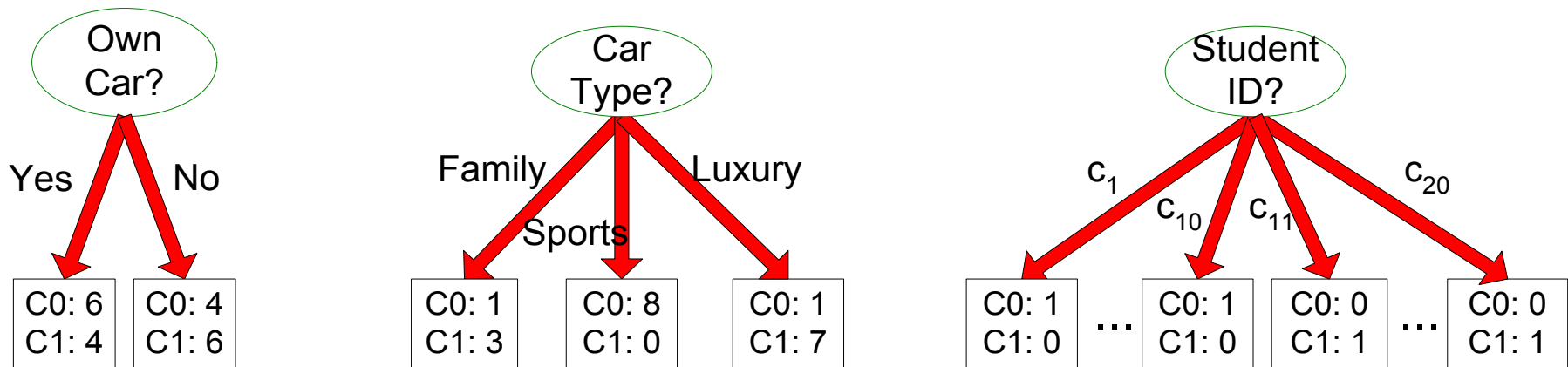
# Tree Induction

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- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - ◆ How to specify the attribute test condition?
    - ◆ How to determine the best split?
  - Determine when to stop splitting

# How to determine the Best Split

Before Splitting: 10 records of class 0,  
10 records of class 1



Which test condition is the best?

# How to determine the Best Split

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- Greedy approach:
  - Nodes with **homogeneous** class distribution are preferred
- Need a measure of node impurity:

C0: 5
C1: 5

**Non-homogeneous,  
High degree of impurity**

C0: 9
C1: 1

**Homogeneous,  
Low degree of impurity**

# Measures of Node Impurity

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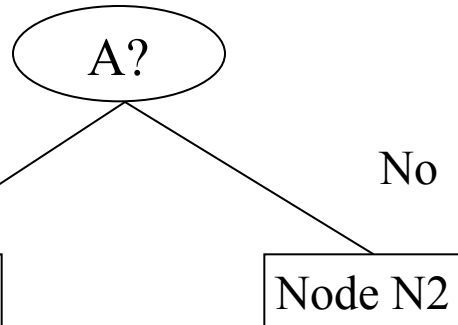
- Gini Index
- Entropy
- Misclassification error

# How to Find the Best Split

Before Splitting:

C0	<b>N00</b>
C1	<b>N01</b>

→ **M0**



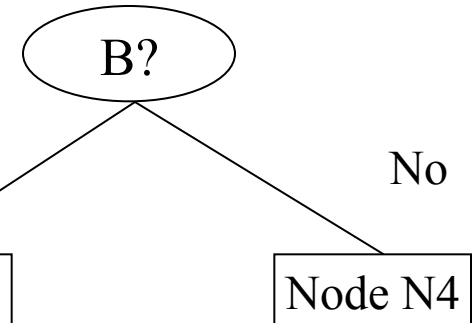
C0	<b>N10</b>
C1	<b>N11</b>

C0	<b>N20</b>
C1	<b>N21</b>

↓  
**M1**

↓  
**M2**

**M12**



C0	<b>N30</b>
C1	<b>N31</b>

C0	<b>N40</b>
C1	<b>N41</b>

↓  
**M3**

↓  
**M4**

**M34**

**Gain = M0 – M12 vs M0 – M34**

# Measure of Impurity: GINI

- Gini Index for a given node  $t$  :

$$GINI(t) = 1 - \sum_j [p(j | t)]^2$$

(NOTE:  $p(j | t)$  is the relative frequency of class  $j$  at node  $t$ ).

- Maximum ( $1 - 1/n_c$ ) when records are equally distributed among all classes, implying least interesting information
- Minimum (0.0) when all records belong to one class, implying most interesting information

C1	<b>0</b>
C2	<b>6</b>
<b>Gini=0.000</b>	

C1	<b>1</b>
C2	<b>5</b>
<b>Gini=0.278</b>	

C1	<b>2</b>
C2	<b>4</b>
<b>Gini=0.444</b>	

C1	<b>3</b>
C2	<b>3</b>
<b>Gini=0.500</b>	

# Examples for computing GINI

$$GINI(t) = 1 - \sum_j [p(j | t)]^2$$

C1	<b>0</b>
C2	<b>6</b>

$$P(C1) = 0/6 = 0 \quad P(C2) = 6/6 = 1$$

$$Gini = 1 - P(C1)^2 - P(C2)^2 = 1 - 0 - 1 = 0$$

C1	<b>1</b>
C2	<b>5</b>

$$P(C1) = 1/6 \quad P(C2) = 5/6$$

$$Gini = 1 - (1/6)^2 - (5/6)^2 = 0.278$$

C1	<b>2</b>
C2	<b>4</b>

$$P(C1) = 2/6 \quad P(C2) = 4/6$$

$$Gini = 1 - (2/6)^2 - (4/6)^2 = 0.444$$



# Splitting Based on GINI

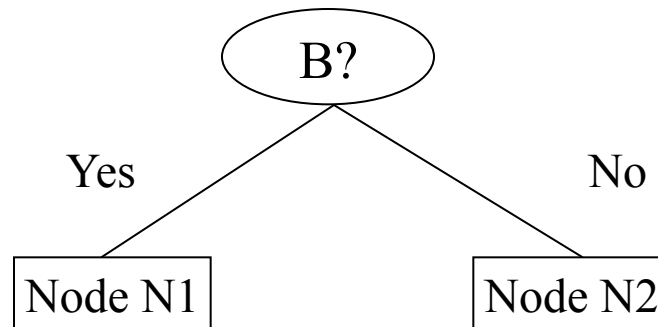
- Used in CART, SLIQ, SPRINT.
- When a node  $p$  is split into  $k$  partitions (children), the quality of split is computed as,

$$GINI_{split} = \sum_{i=1}^k \frac{n_i}{n} GINI(i)$$

where,  $n_i$  = number of records at child  $i$ ,  
 $n$  = number of records at node  $p$ .

# Binary Attributes: Computing GINI Index

- Splits into two partitions
- Effect of Weighing partitions:
  - Larger and Purer Partitions are sought for.



	Parent
C1	<b>6</b>
C2	<b>6</b>
<b>Gini = 0.500</b>	

$$\begin{aligned}
 \text{Gini}(N1) &= 1 - (5/6)^2 - (2/6)^2 \\
 &= 0.194
 \end{aligned}$$

$$\begin{aligned}
 \text{Gini}(N2) &= 1 - (1/6)^2 - (4/6)^2 \\
 &= 0.528
 \end{aligned}$$

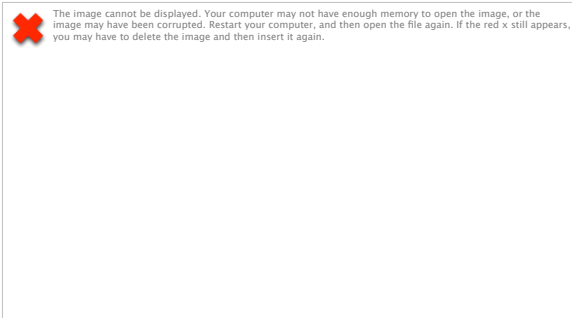
	N1	N2
C1	<b>5</b>	<b>1</b>
C2	<b>2</b>	<b>4</b>
<b>Gini=0.333</b>		

$$\begin{aligned}
 \text{Gini(Children)} &= 7/12 * 0.194 + \\
 &\quad 5/12 * 0.528 \\
 &= 0.333
 \end{aligned}$$

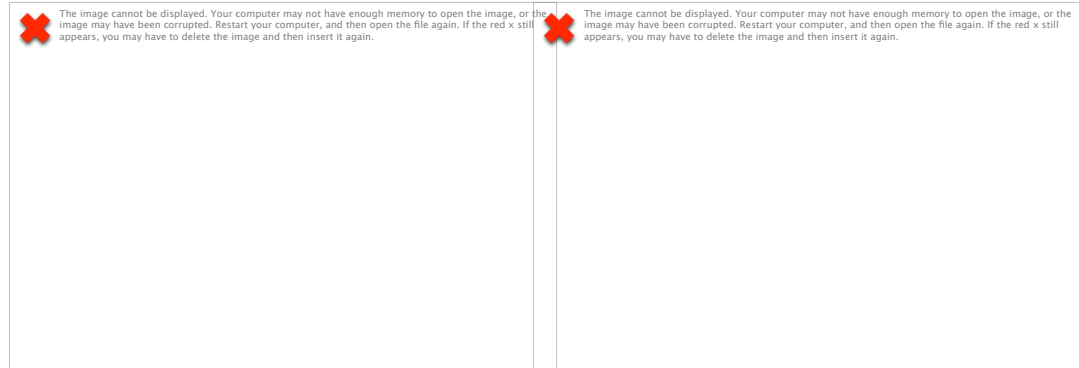
# Categorical Attributes: Computing Gini Index

- For each distinct value, gather counts for each class in the dataset
- Use the count matrix to make decisions

Multi-way split



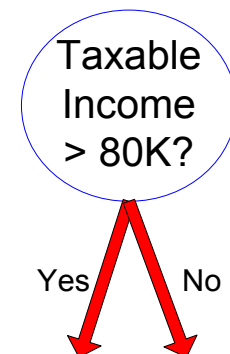
Two-way split  
(find best partition of values)



# Continuous Attributes: Computing Gini Index

- Use Binary Decisions based on one value
- Several Choices for the splitting value
  - Number of possible splitting values = Number of distinct values
- Each splitting value has a count matrix associated with it
  - Class counts in each of the partitions,  $A < v$  and  $A \geq v$
- Simple method to choose best  $v$ 
  - For each  $v$ , scan the database to gather count matrix and compute its Gini index
  - Computationally Inefficient! Repetition of work.

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8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



# Continuous Attributes: Computing Gini Index...

- For efficient computation: for each attribute,
  - Sort the attribute on values
  - Linearly scan these values, each time updating the count matrix and computing gini index
  - Choose the split position that has the least gini index

		Cheat	No		No		No		Yes		Yes		Yes		No		No		No		No			
			Taxable Income																					
Sorted Values	→	60		70		75		85		90		95		100		120		125		220				
		55		65		72		80		87		92		97		110		122		172		230		
Split Positions	→	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	
		Yes	0	3	0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	3	0
		No	0	7	1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	7	0
		Gini	0.420		0.400		0.375		0.343		0.417		0.400		<u>0.300</u>		0.343		0.375		0.400		0.420	

# Alternative Splitting Criteria based on INFO

- Entropy at a given node t:

$$Entropy(t) = -\sum_j p(j | t) \log p(j | t)$$

(NOTE:  $p(j | t)$  is the relative frequency of class j at node t).

- Measures homogeneity of a node.
  - ◆ Maximum ( $\log n_c$ ) when records are equally distributed among all classes implying least information
  - ◆ Minimum (0.0) when all records belong to one class, implying most information
- Entropy based computations are similar to the GINI index computations

# Examples for computing Entropy

$$Entropy(t) = -\sum_j p(j | t) \log_2 p(j | t)$$

C1	<b>0</b>
C2	<b>6</b>

$$P(C1) = 0/6 = 0 \quad P(C2) = 6/6 = 1$$

$$Entropy = -0 \log 0 - 1 \log 1 = -0 - 0 = 0$$

C1	<b>1</b>
C2	<b>5</b>

$$P(C1) = 1/6 \quad P(C2) = 5/6$$

$$Entropy = - (1/6) \log_2 (1/6) - (5/6) \log_2 (1/6) = 0.65$$

C1	<b>2</b>
C2	<b>4</b>

$$P(C1) = 2/6 \quad P(C2) = 4/6$$

$$Entropy = - (2/6) \log_2 (2/6) - (4/6) \log_2 (4/6) = 0.92$$

# Splitting Based on INFO...

- Information Gain:

$$GAIN_{split} = Entropy(p) - \left( \sum_{i=1}^k \frac{n_i}{n} Entropy(i) \right)$$

Parent Node, p is split into k partitions;

$n_i$  is number of records in partition i

- Measures Reduction in Entropy achieved because of the split. Choose the split that achieves most reduction (maximizes GAIN)
- Used in ID3 and C4.5
- Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.



# Splitting Based on INFO...

- Gain Ratio:

$$GainRATIO_{split} = \frac{GAIN_{Split}}{SplitINFO} \quad SplitINFO = -\sum_{i=1}^k \frac{n_i}{n} \log \frac{n_i}{n}$$

Parent Node, p is split into k partitions

$n_i$  is the number of records in partition i

- Adjusts Information Gain by the entropy of the partitioning (SplitINFO). Higher entropy partitioning (large number of small partitions) is penalized!
- Used in C4.5
- Designed to overcome the disadvantage of Information Gain

# Splitting Criteria based on Classification Error

- Classification error at a node  $t$  :

$$Error(t) = 1 - \max_i P(i | t)$$

- Measures misclassification error made by a node.
  - ◆ Maximum  $(1 - 1/n_c)$  when records are equally distributed among all classes, implying least interesting information
  - ◆ Minimum (0.0) when all records belong to one class, implying most interesting information

# Examples for Computing Error

$$Error(t) = 1 - \max_i P(i | t)$$

C1	<b>0</b>
C2	<b>6</b>

$$P(C1) = 0/6 = 0 \quad P(C2) = 6/6 = 1$$

$$Error = 1 - \max(0, 1) = 1 - 1 = 0$$

C1	<b>1</b>
C2	<b>5</b>

$$P(C1) = 1/6 \quad P(C2) = 5/6$$

$$Error = 1 - \max(1/6, 5/6) = 1 - 5/6 = 1/6$$

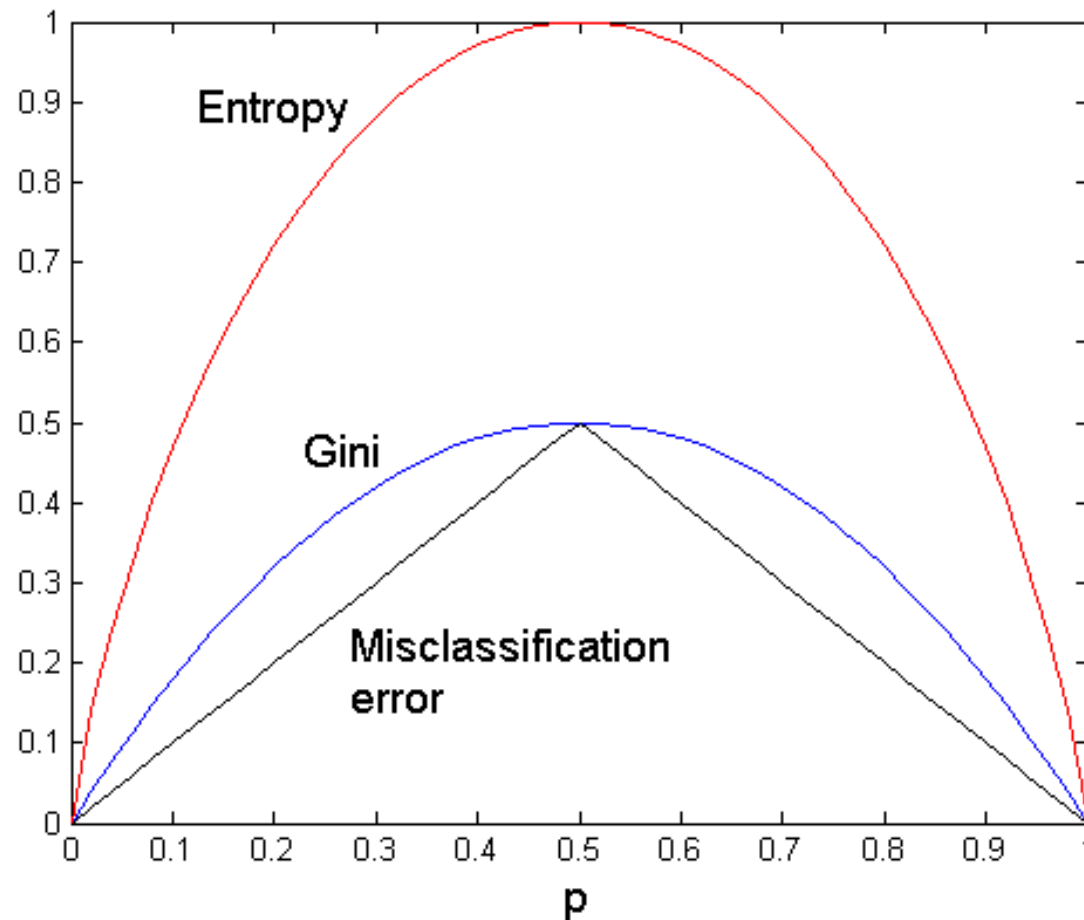
C1	<b>2</b>
C2	<b>4</b>

$$P(C1) = 2/6 \quad P(C2) = 4/6$$

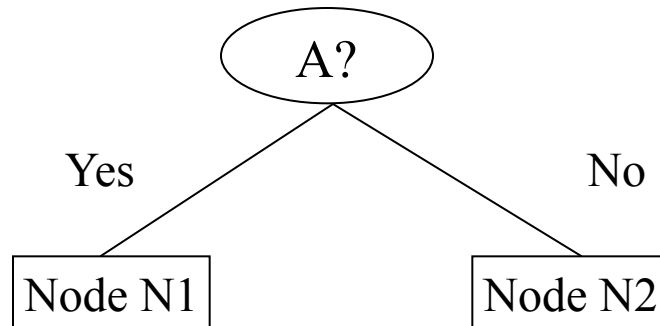
$$Error = 1 - \max(2/6, 4/6) = 1 - 4/6 = 1/3$$

# Comparison among Splitting Criteria

For a 2-class problem:



# Misclassification Error vs Gini



	Parent
C1	<b>7</b>
C2	<b>3</b>
<b>Gini = 0.42</b>	

$$\begin{aligned}
 &\text{Gini(N1)} \\
 &= 1 - (3/3)^2 - (0/3)^2 \\
 &= 0
 \end{aligned}$$

	N1	N2
C1	<b>3</b>	<b>4</b>
C2	<b>0</b>	<b>3</b>
<b>Gini=0.361</b>		

$$\begin{aligned}
 &\text{Gini(N2)} \\
 &= 1 - (4/7)^2 - (3/7)^2 \\
 &= 0.489
 \end{aligned}$$

$$\begin{aligned}
 &\text{Gini(Children)} \\
 &= 3/10 * 0 \\
 &+ 7/10 * 0.489 \\
 &= 0.342
 \end{aligned}$$

**Gini improves !!**

# Tree Induction

---

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - ◆ How to specify the attribute test condition?
    - ◆ How to determine the best split?
  - Determine when to stop splitting

# Stopping Criteria for Tree Induction

---

- Stop expanding a node when all the records belong to the same class
- Stop expanding a node when all the records have similar attribute values
- Early termination (to be discussed later)

# Decision Tree Based Classification

---

- Advantages:
  - Inexpensive to construct
  - Extremely fast at classifying unknown records
  - Easy to interpret for small-sized trees
  - Accuracy is comparable to other classification techniques for many simple data sets



# Example: C4.5

---

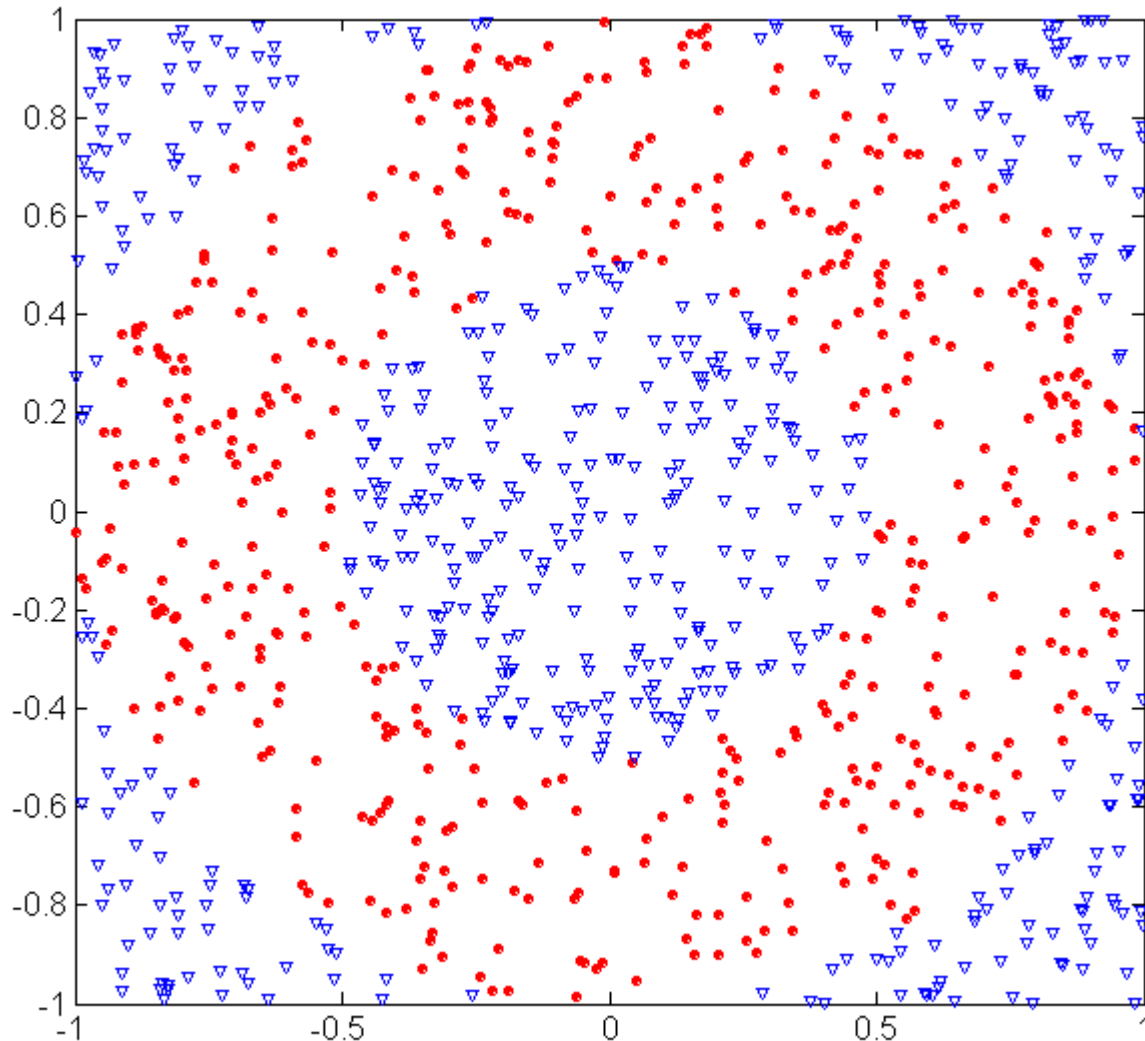
- Simple depth-first construction.
- Uses Information Gain
- Sorts Continuous Attributes at each node.
- Needs entire data to fit in memory.
- Unsuitable for Large Datasets.
  - Needs out-of-core sorting.
- You can download the software from:  
<http://www.cse.unsw.edu.au/~quinlan/c4.5r8.tar.gz>

# Practical Issues of Classification

---

- Underfitting and Overfitting
- Missing Values
- Costs of Classification

# Underfitting and Overfitting (Example)



**500 circular and 500 triangular data points.**

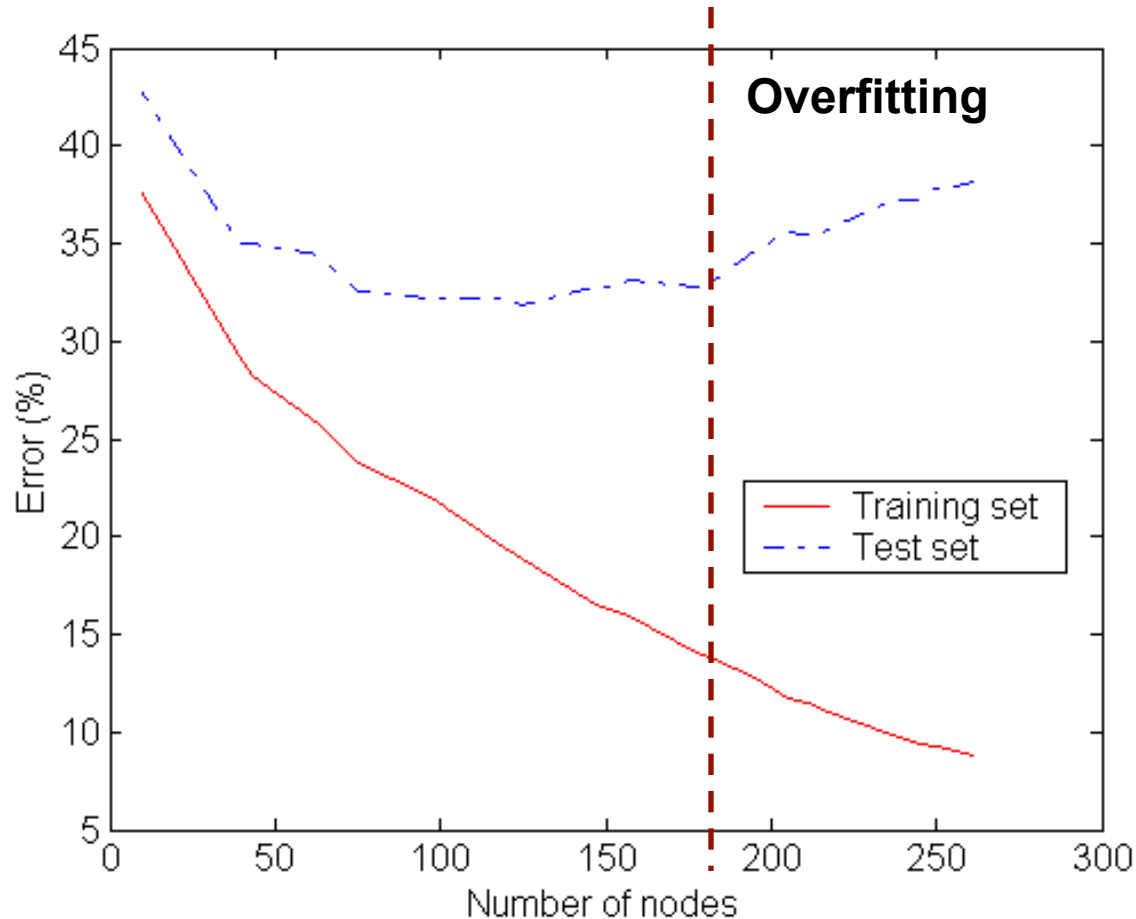
**Circular points:**

$$0.5 \leq \text{sqrt}(x_1^2 + x_2^2) \leq 1$$

**Triangular points:**

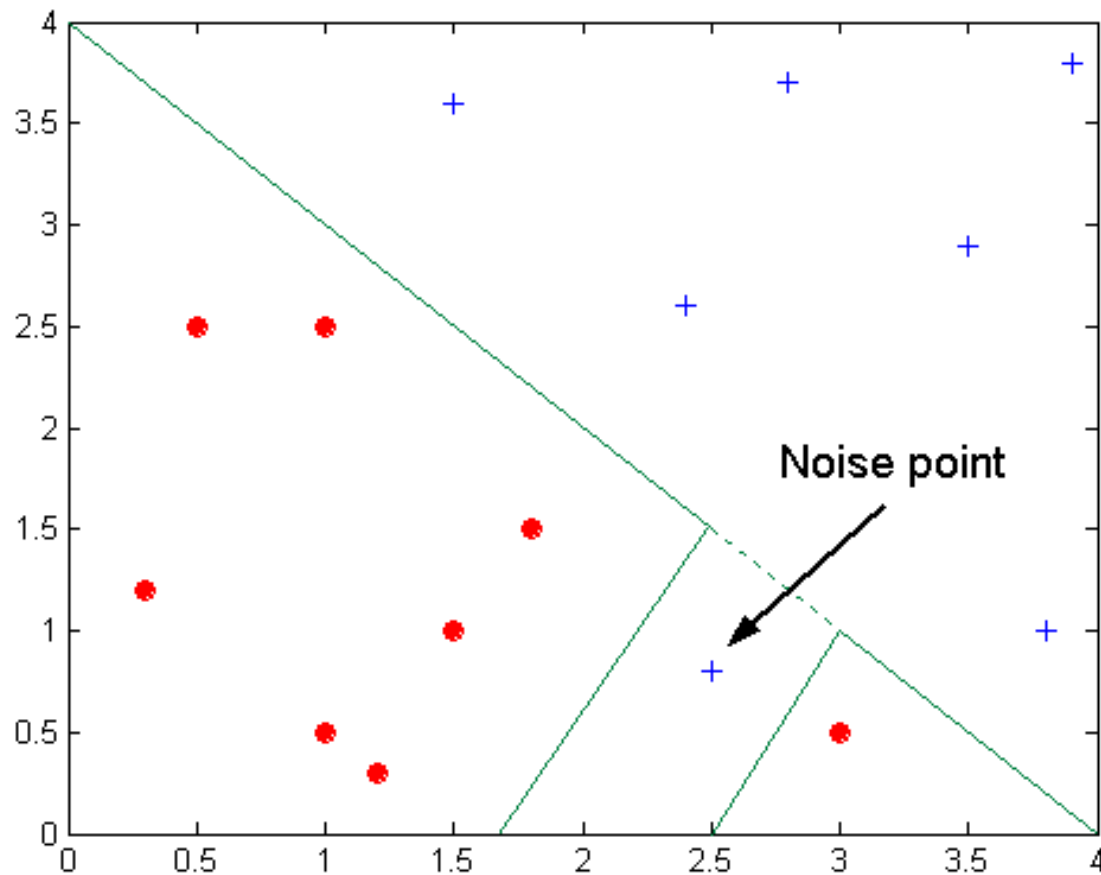
$$\text{sqrt}(x_1^2 + x_2^2) > 0.5 \text{ or } \text{sqrt}(x_1^2 + x_2^2) < 1$$

# Underfitting and Overfitting



**Underfitting:** when model is too simple, both training and test errors are large

# Overfitting due to Noise



**Decision boundary is distorted by noise point**

# Overfitting due to Noise

**Table 4.4.** An example test set for classifying mammals.

Name	Body Temperature	Gives Birth	Four-legged	Hibernates	Class Label
human	warm-blooded	yes	no	no	yes
pigeon	warm-blooded	no	no	no	no
elephant	warm-blooded	yes	yes	no	yes
leopard shark	cold-blooded	yes	no	no	no
turtle	cold-blooded	no	yes	no	no
penguin	cold-blooded	no	no	no	no
eel	cold-blooded	no	no	no	no
dolphin	warm-blooded	yes	no	no	yes
spiny anteater	warm-blooded	no	yes	yes	yes
gila monster	cold-blooded	no	yes	yes	no

\* Bats and Whales are misclassified; non-mammals instead of mammals.

# Overfitting due to Noise

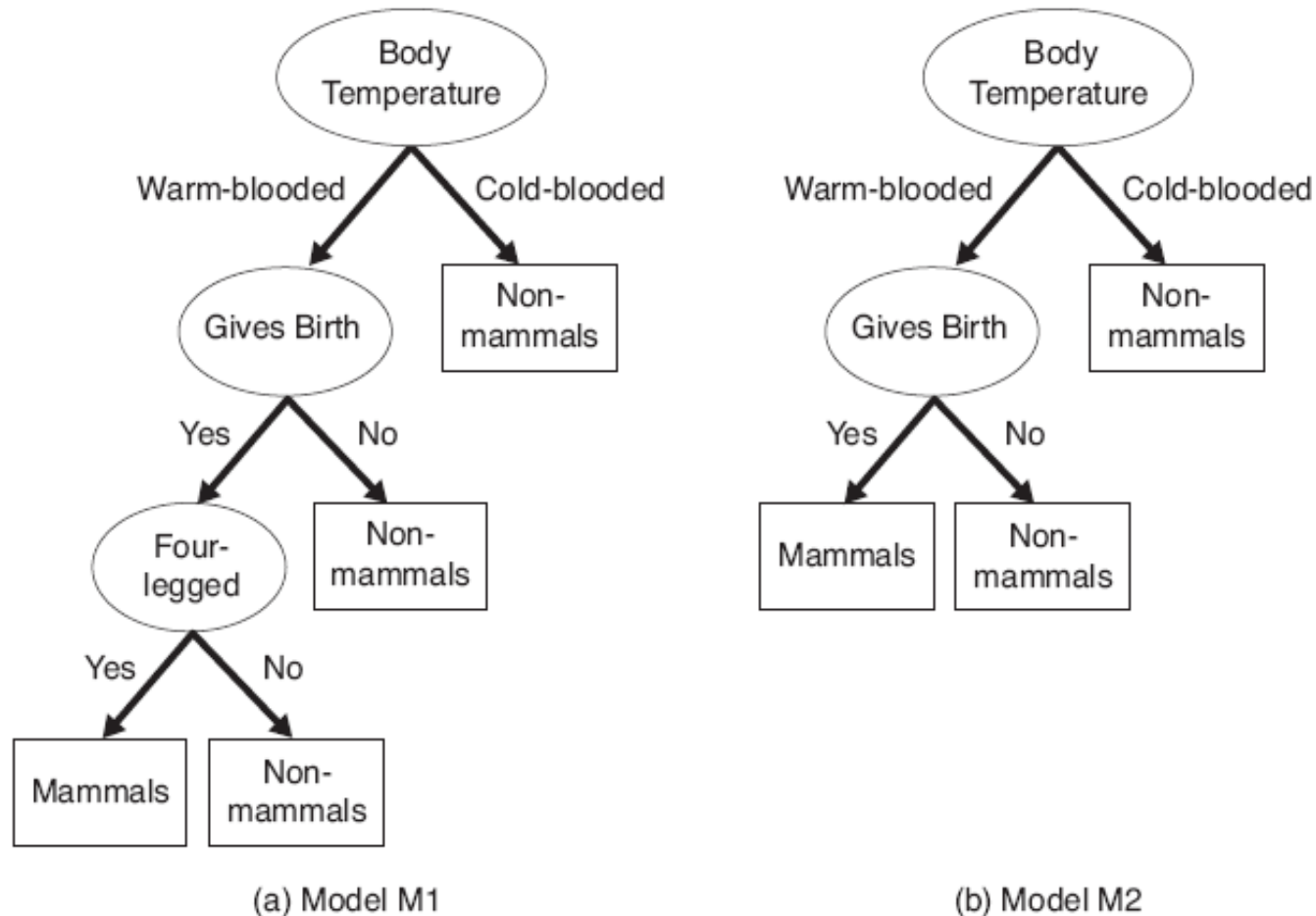


Figure 4.25. Decision tree induced from the data set shown in Table 4.3.

# Overfitting due to Noise

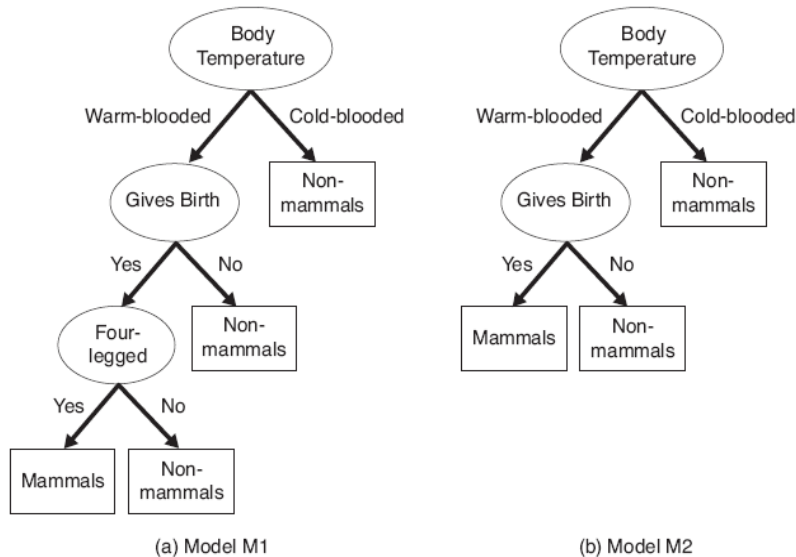


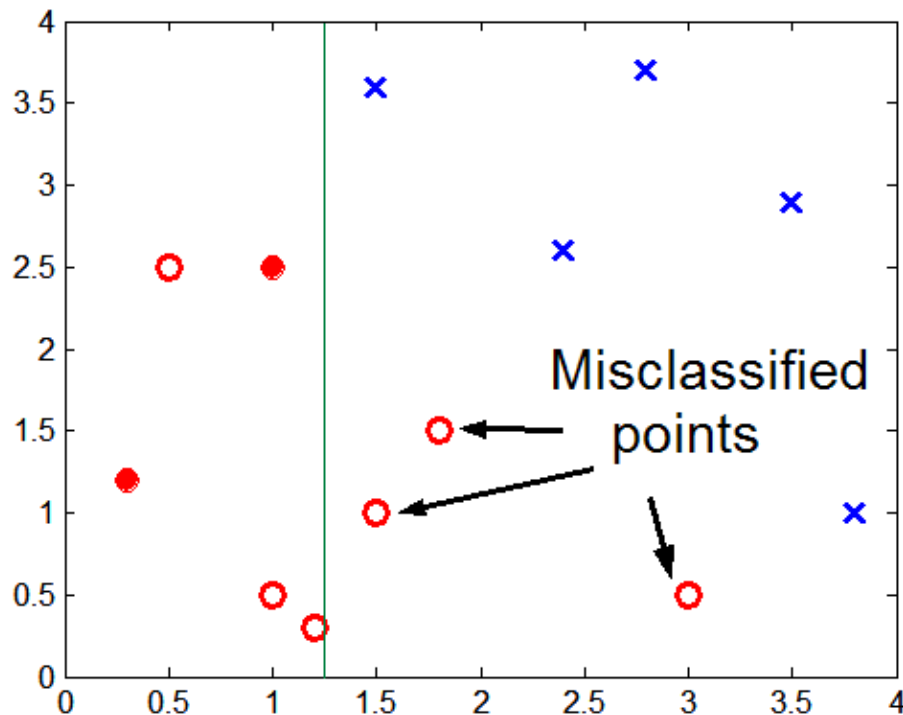
Figure 4.25. Decision tree induced from the data set shown in Table 4.3.

- Decision tree perfectly fits training data (training error=0)
- But error rate on test data is 30%.

- Both humans and dolphins were misclassified as non-mammals b/c Body Temp, Gives\_Birth and Four-legged values are identical to mislabeled records in training set.
- Spiny anteaters represent an exceptional case (every warm-blooded with no gives\_birth is non-mammal in TR\_Set)



# Overfitting due to Insufficient Examples



**Lack of data points in the lower half of the diagram makes it difficult to predict correctly the class labels of that region**

- Insufficient number of training records in the region causes the decision tree to predict the test examples using other training records that are irrelevant to the classification task**

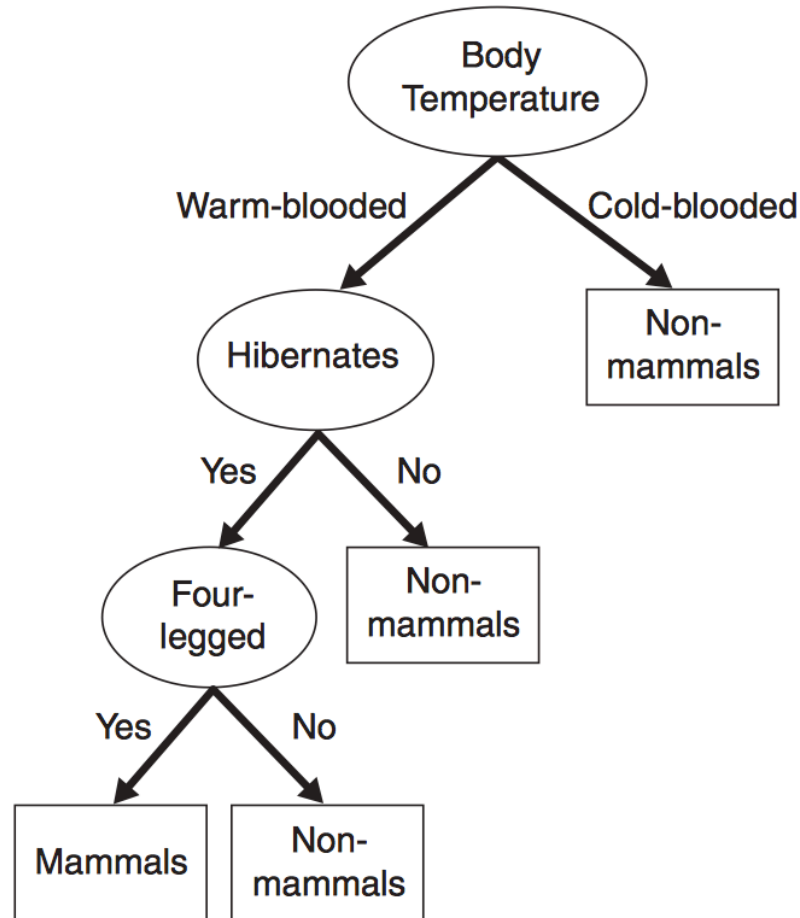
# Overfitting due to Insufficient Examples

**Table 4.5.** An example training set for classifying mammals.

Name	Body Temperature	Gives Birth	Four-legged	Hibernates	Class Label
salamander	cold-blooded	no	yes	yes	no
guppy	cold-blooded	yes	no	no	no
eagle	warm-blooded	no	no	no	no
poorwill	warm-blooded	no	no	yes	no
platypus	warm-blooded	no	yes	yes	yes

Models that make their classification decisions based on a small number of training records are also susceptible to overfitting.

# Overfitting due to Insufficient Examples



**Figure 4.26.** Decision tree induced from the data set shown in Table 4.5.

# Overfitting due to Insufficient Examples

---

- All of these training records are labeled correctly and its training error is zero, its error rate on the test set is 30%.
- Humans, elephants, and dolphins are misclassified because the decision tree classifies all warm-blooded vertebrates that do not hibernate as non-mammals.
- The tree arrives at this classification decision because there is only one training record, which is an eagle, with such characteristics.
- This example clearly demonstrates the danger of making wrong predictions when there are not enough representative examples at the leaf nodes of a decision tree.

# Notes on Overfitting

---

- Overfitting results in decision trees that are more complex than necessary
- Training error no longer provides a good estimate of how well the tree will perform on previously unseen records
- Need new ways for estimating errors

# Estimating Generalization Errors

- **Re-substitution errors:** error on training ( $\sum e(t)$  )
- **Generalization errors:** error on testing ( $\sum e'(t)$ )
- Methods for estimating generalization errors:
  - **Optimistic approach:**  $e'(t) = e(t)$
  - **Pessimistic approach:**
    - ◆ For each leaf node:  $e'(t) = (e(t)+0.5)$
    - ◆ Total errors:  $e'(T) = e(T) + N \times 0.5$  (N: number of leaf nodes)
    - ◆ For a tree with 30 leaf nodes and 10 errors on training (out of 1000 instances):  
Training error =  $10/1000 = 1\%$   
Generalization error =  $(10 + 30 \times 0.5)/1000 = 2.5\%$
  - **Reduced error pruning (REP):**
    - ◆ uses validation data set to estimate generalization error

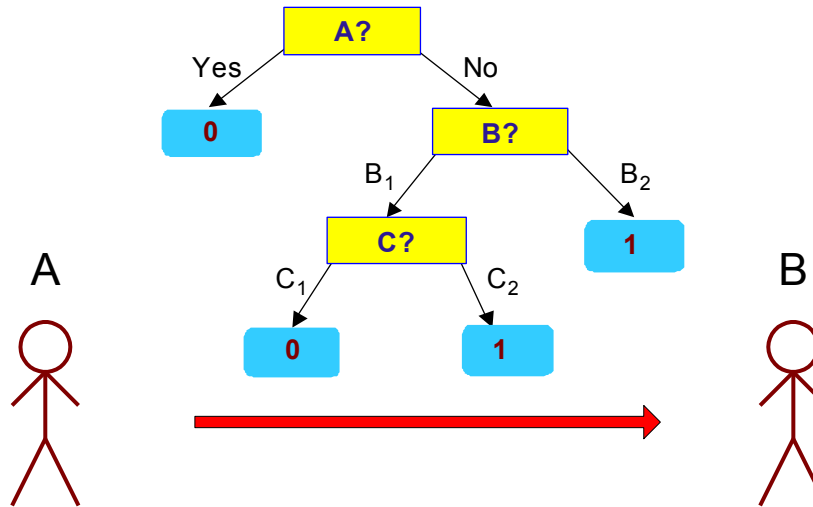
# Occam's Razor

---

- Given two models of similar generalization errors, one should prefer the simpler model over the more complex model
- For complex models, there is a greater chance that it was fitted accidentally by errors in data
- Therefore, one should include model complexity when evaluating a model

# Minimum Description Length (MDL)

X	y
X <sub>1</sub>	1
X <sub>2</sub>	0
X <sub>3</sub>	0
X <sub>4</sub>	1
...	...
X <sub>n</sub>	1



X	y
X <sub>1</sub>	?
X <sub>2</sub>	?
X <sub>3</sub>	?
X <sub>4</sub>	?
...	...
X <sub>n</sub>	?

- $\text{Cost}(\text{Model}, \text{Data}) = \text{Cost}(\text{Data} | \text{Model}) + \text{Cost}(\text{Model})$ 
  - Cost is the number of bits needed for encoding.
  - Search for the least costly model.
- $\text{Cost}(\text{Data} | \text{Model})$  encodes the misclassification errors.
- $\text{Cost}(\text{Model})$  uses node encoding (number of children) plus splitting condition encoding.



# How to Address Overfitting

---

- Pre-Pruning (Early Stopping Rule)

- Stop the algorithm before it becomes a fully-grown tree
- Typical stopping conditions for a node:
  - ◆ Stop if all instances belong to the same class
  - ◆ Stop if all the attribute values are the same
- More restrictive conditions:
  - ◆ Stop if number of instances is less than some user-specified threshold
  - ◆ Stop if class distribution of instances are independent of the available features (e.g., using  $\chi^2$  test)
  - ◆ Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain).

# How to Address Overfitting...

---

- Post-pruning

- Grow decision tree to its entirety
- Trim the nodes of the decision tree in a bottom-up fashion
- If generalization error improves after trimming, replace sub-tree by a leaf node.
- Class label of leaf node is determined from majority class of instances in the sub-tree
- Can use MDL for post-pruning

# Example of Post-Pruning

Class = Yes	20
Class = No	10
Error = 10/30	

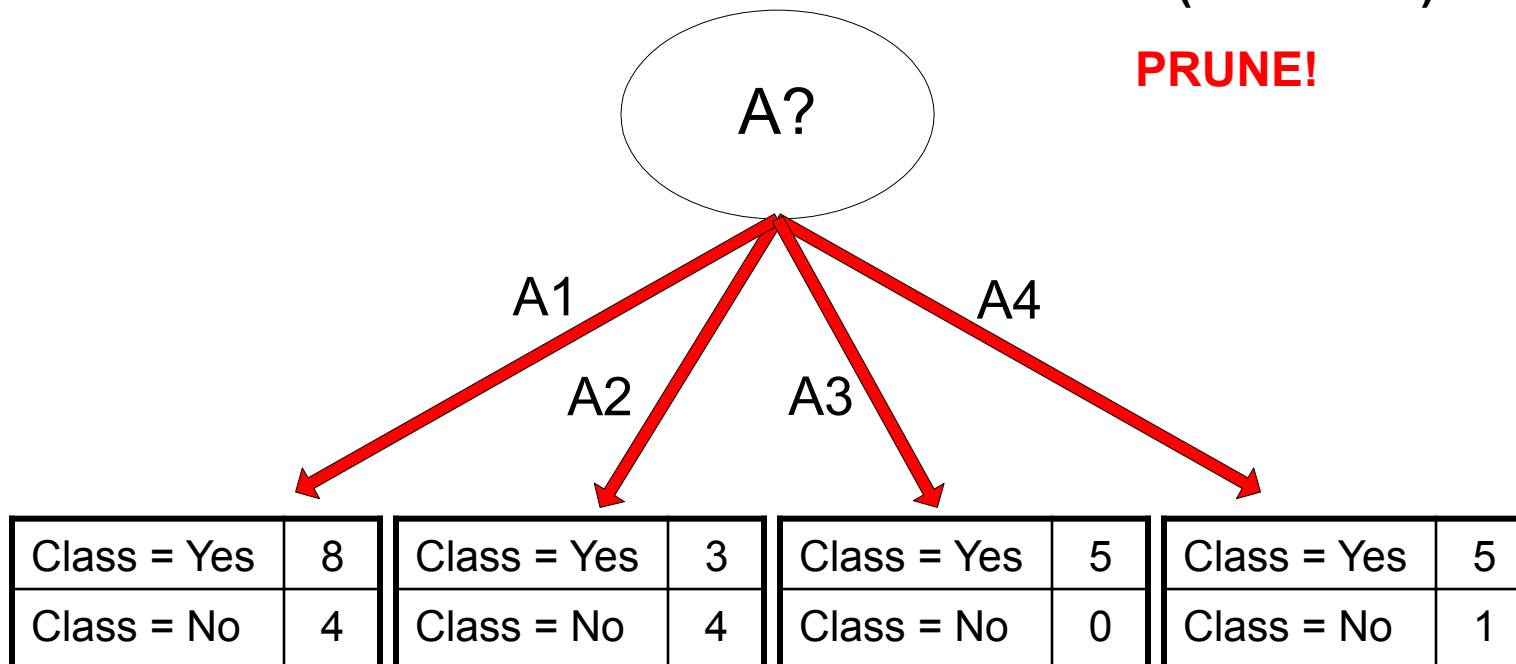
Training Error (Before splitting) = 10/30

Pessimistic error =  $(10 + 0.5)/30 = 10.5/30$

Training Error (After splitting) = 9/30

Pessimistic error (After splitting)  
 $= (9 + 4 \times 0.5)/30 = 11/30$

**PRUNE!**



# Examples of Post-pruning

- Optimistic error?

Don't prune for both cases

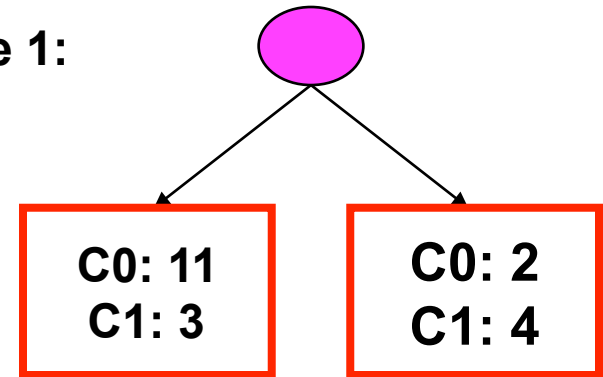
- Pessimistic error?

Don't prune case 1, prune case 2

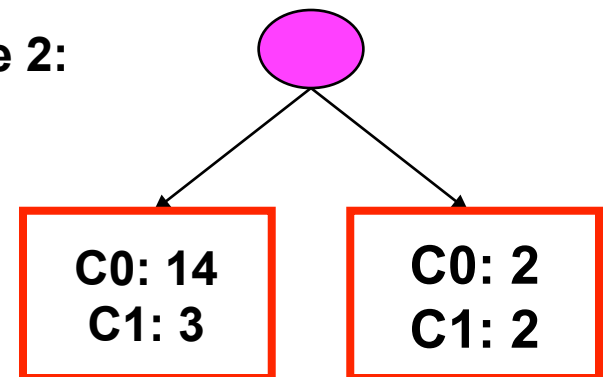
- Reduced error pruning?

Depends on validation set

Case 1:



Case 2:



# Handling Missing Attribute Values

---

- Missing values affect decision tree construction in three different ways:
  - Affects how impurity measures are computed
  - Affects how to distribute instance with missing value to child nodes
  - Affects how a test instance with missing value is classified

# Computing Impurity Measure

<i>Tid</i>	Refund	Marital Status	Taxable Income	Class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	?	Single	90K	Yes

Missing  
value

**Before Splitting:**

Entropy(Parent)

$$= -0.3 \log(0.3) - (0.7) \log(0.7) = 0.8813$$

	Class = Yes	Class = No
Refund=Yes	0	3
Refund=No	2	4
Refund=?	1	0

**Split on Refund:**

Entropy(Refund=Yes) = 0

Entropy(Refund=No)

$$= -(2/6) \log(2/6) - (4/6) \log(4/6) = 0.9183$$

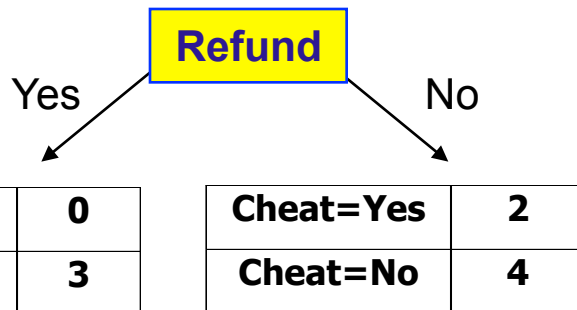
Entropy(Children)

$$= 0.3 (0) + 0.6 (0.9183) = 0.551$$

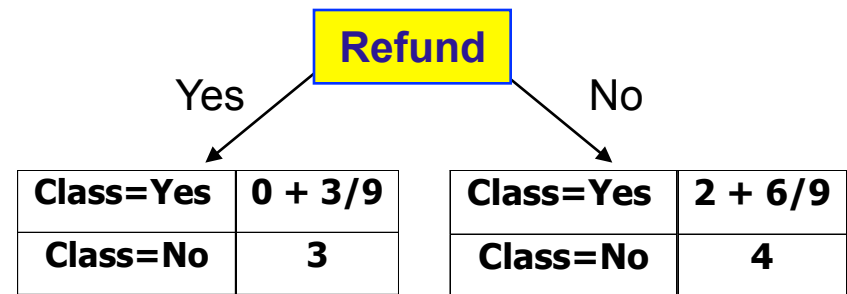
$$\text{Gain} = 0.9 \times (0.8813 - 0.551) = 0.3303$$

# Distribute Instances

Tid	Refund	Marital Status	Taxable Income	Class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No



Tid	Refund	Marital Status	Taxable Income	Class
10	?	Single	90K	Yes



Probability that Refund=Yes is 3/9

Probability that Refund=No is 6/9

Assign record to the left child with weight = 3/9 and to the right child with weight = 6/9

# Exam I Review

---

- What is Data Mining?
- Application of Data Mining in Various Domains and Cases?
- Types of Data?
- Why to know your data is important?
- Sampling, Aggregation,...
- Curse of Dimensionality
- Similarity calculations (expect 1 question)
- Interpreting visualizations
- Basics of PCA



# Exam I Review

---

- Classification: Accuracy vs Error Rate
- Entropy, Gini, Error & Gain calculations
- Overfitting concepts: what, why, how
- Generalization errors (pessimistic/optimistic)

# Data Fragmentation

---

- Number of instances gets smaller as you traverse down the tree
- Number of instances at the leaf nodes could be too small to make any statistically significant decision

# Other Issues

---

- Data Fragmentation
- Search Strategy
- Expressiveness
- Tree Replication

# Search Strategy

---

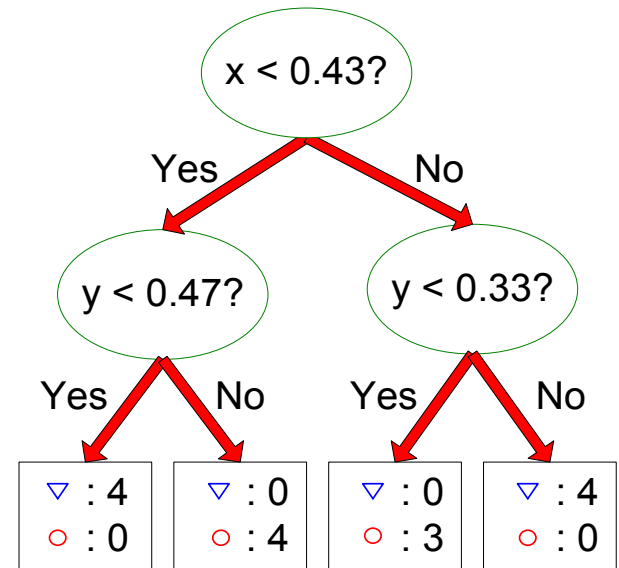
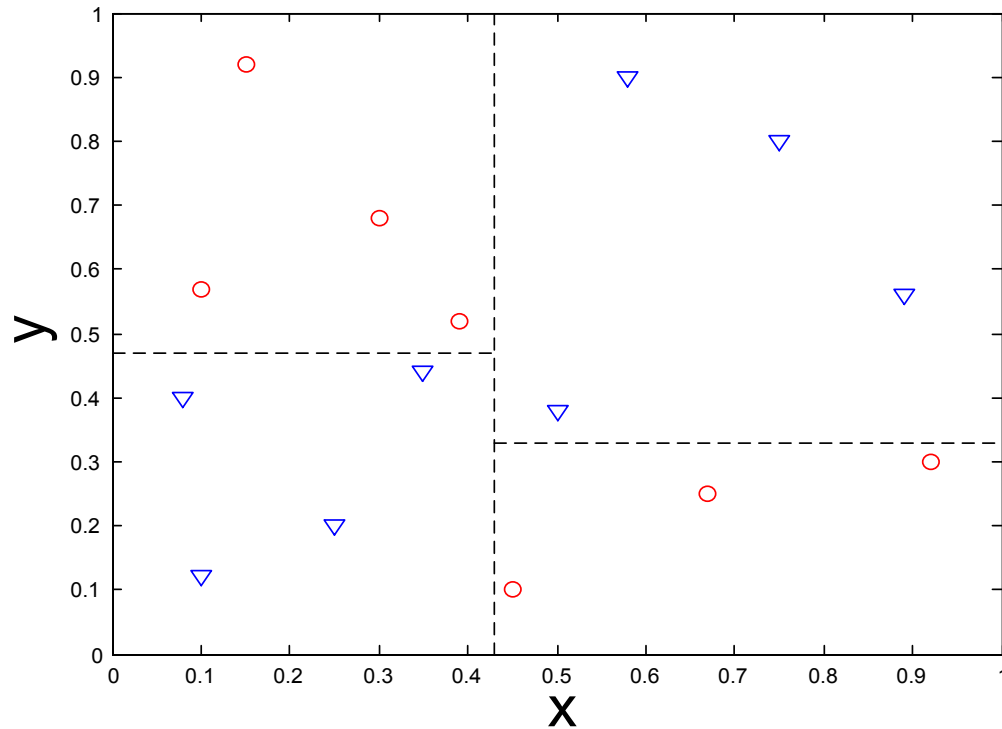
- Finding an optimal decision tree is NP-hard
- The algorithm presented so far uses a greedy, top-down, recursive partitioning strategy to induce a reasonable solution
- Other strategies?
  - Bottom-up
  - Bi-directional

# Expressiveness

---

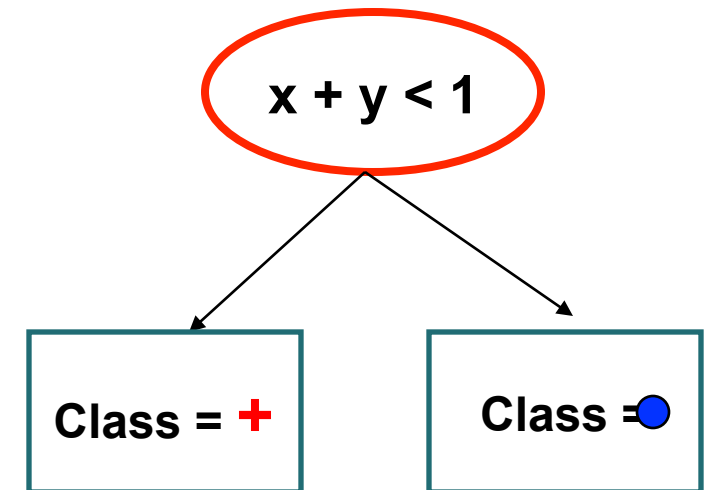
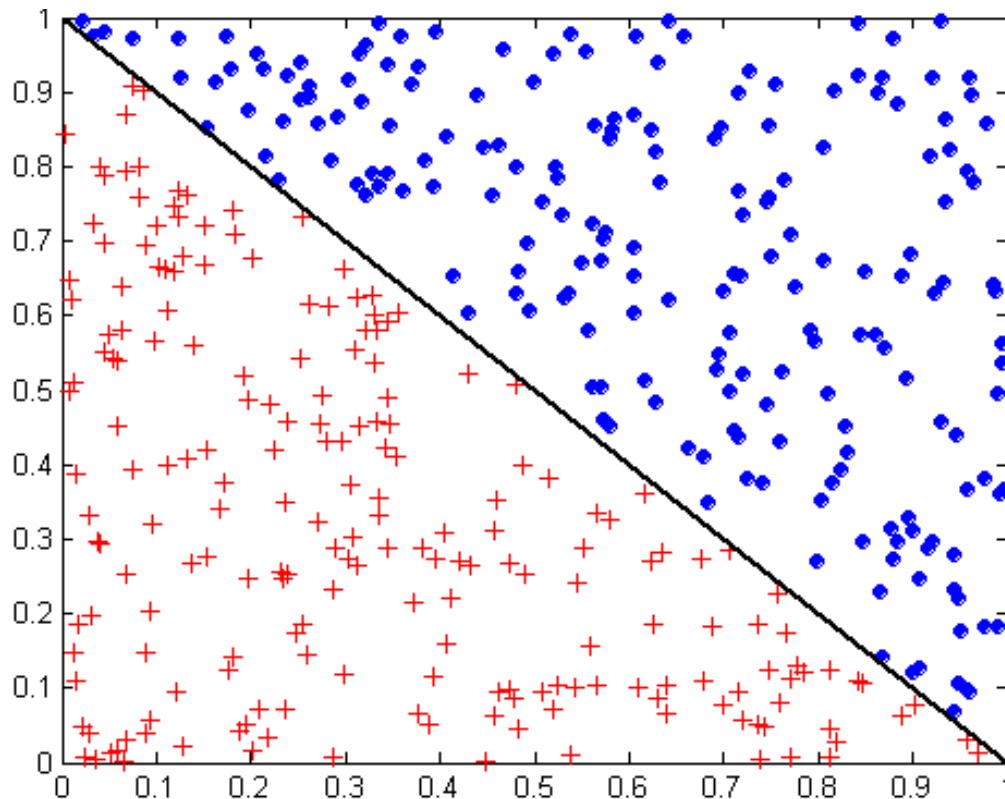
- Decision tree provides expressive representation for learning discrete-valued function
  - But they do not generalize well to certain types of Boolean functions
    - ◆ Example: parity function:
      - Class = 1 if there is an even number of Boolean attributes with truth value = True
      - Class = 0 if there is an odd number of Boolean attributes with truth value = True
    - ◆ For accurate modeling, must have a complete tree
- Not expressive enough for modeling continuous variables
  - Particularly when test condition involves only a single attribute at-a-time

# Decision Boundary



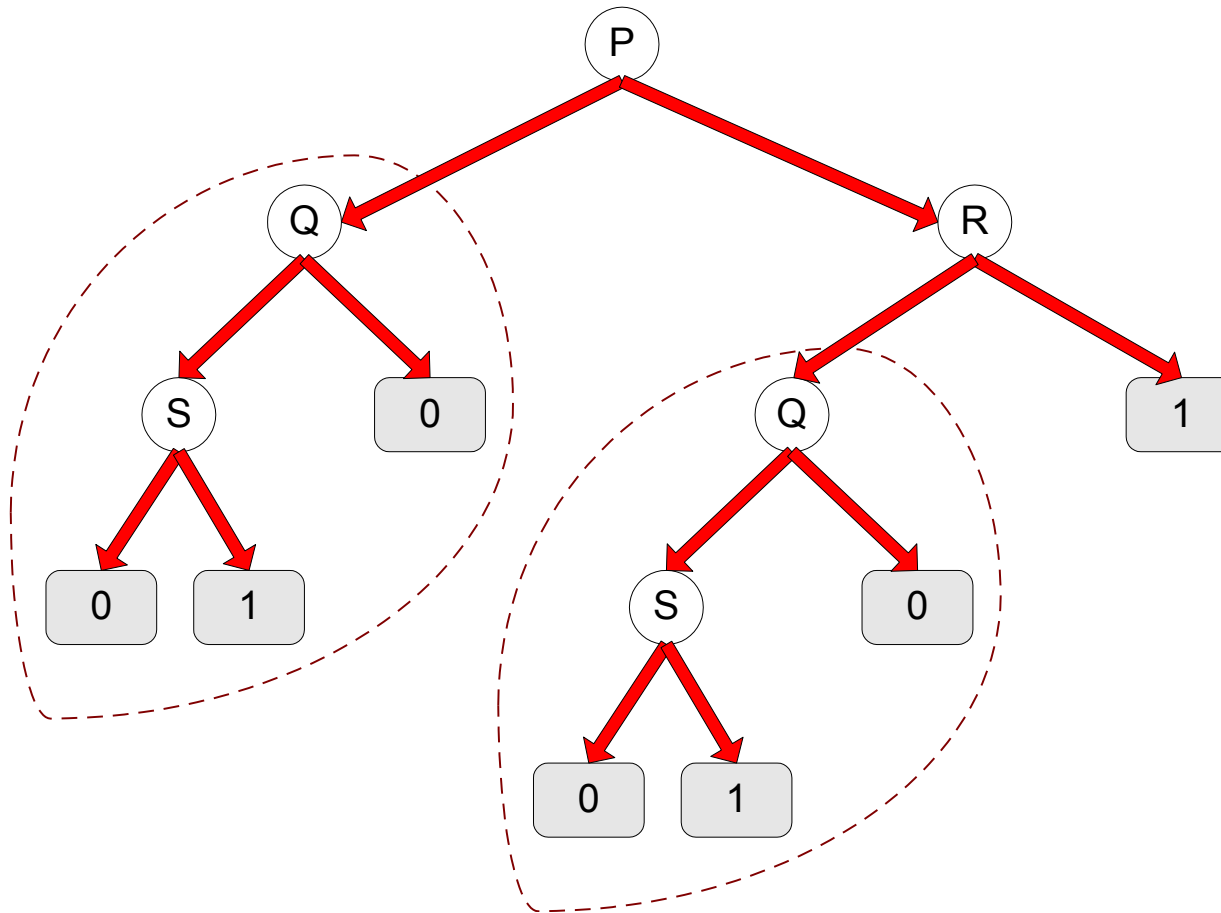
- Border line between two neighboring regions of different classes is known as decision boundary
- Decision boundary is parallel to axes because test condition involves a single attribute at-a-time

# Oblique Decision Trees



- Test condition may involve multiple attributes
- More expressive representation
- Finding optimal test condition is computationally expensive

# Tree Replication



- Same subtree appears in multiple branches



# Model Evaluation

---

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Model Comparison
  - How to compare the relative performance among competing models?

# Model Evaluation

---

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Model Comparison
  - How to compare the relative performance among competing models?

# Metrics for Performance Evaluation

- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

	PREDICTED CLASS		
		Class=Yes	Class=No
	Class=Yes	a	b
ACTUAL CLASS	Class=No	c	d

a: TP (true positive)  
b: FN (false negative)  
c: FP (false positive)  
d: TN (true negative)

# Metrics for Performance Evaluation...

ACTUAL CLASS	PREDICTED CLASS	
	Class=Yes	Class=No
Class=Yes	a (TP)	b (FN)
	c (FP)	d (TN)

- Most widely-used metric:

$$\text{Accuracy} = \frac{a + d}{a + b + c + d} = \frac{TP + TN}{TP + TN + FP + FN}$$

# Limitation of Accuracy

---

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10
- If model predicts everything to be class 0, accuracy is  $9990/10000 = 99.9\%$ 
  - Accuracy is misleading because model does not detect any class 1 example

# Cost Matrix

	PREDICTED CLASS		
	$C(i j)$	Class=Yes	Class=No
	Class=Yes	$C(\text{Yes} \text{Yes})$	$C(\text{No} \text{Yes})$
	Class=No	$C(\text{Yes} \text{No})$	$C(\text{No} \text{No})$

$C(i|j)$ : Cost of misclassifying class  $j$  example as class  $i$

# Computing Cost of Classification

Cost Matrix	PREDICTED CLASS		
ACTUAL CLASS	C(i j)	+	-
	+	-1	100
	-	1	0

Model $M_1$	PREDICTED CLASS		
ACTUAL CLASS		+	-
	+	150	40
	-	60	250

Accuracy = 80%  
Cost = 3910

Model $M_2$	PREDICTED CLASS		
ACTUAL CLASS		+	-
	+	250	45
	-	5	200

Accuracy = 90%  
Cost = 4255

# Cost vs Accuracy

Count	PREDICTED CLASS		
		Class=Yes	Class=No
	Class=Yes	a	b
	Class=No	c	d

Accuracy is proportional to cost if

1.  $C(\text{Yes}|\text{No})=C(\text{No}|\text{Yes}) = q$
2.  $C(\text{Yes}|\text{Yes})=C(\text{No}|\text{No}) = p$

$$N = a + b + c + d$$

$$\text{Accuracy} = (a + d)/N$$

Cost	PREDICTED CLASS		
		Class=Yes	Class=No
	Class=Yes	p	q
	Class=No	q	p

$$\text{Cost} = p (a + d) + q (b + c)$$

$$= p (a + d) + q (N - a - d)$$

$$= q N - (q - p)(a + d)$$

$$= N [q - (q - p) \times \text{Accuracy}]$$



# Model Evaluation

---

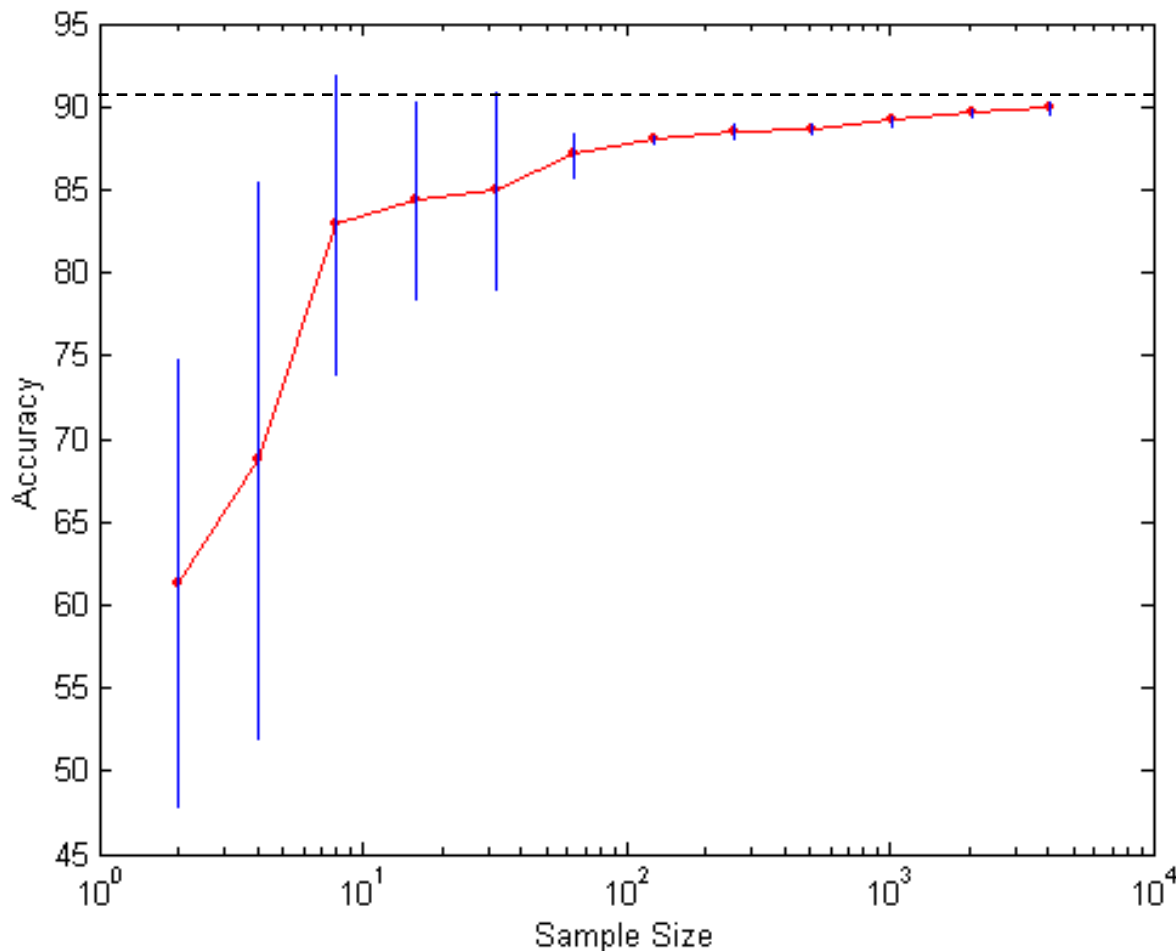
- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Model Comparison
  - How to compare the relative performance among competing models?

# Methods for Performance Evaluation

---

- How to obtain a reliable estimate of performance?
- Performance of a model may depend on other factors besides the learning algorithm:
  - Class distribution
  - Cost of misclassification
  - Size of training and test sets

# Learning Curve



- Learning curve shows how accuracy changes with varying sample size
- Requires a sampling schedule for creating learning curve:
  - Arithmetic sampling (Langley, et al)
  - Geometric sampling (Provost et al)

Effect of small sample size:

- Bias in the estimate
- Variance of estimate

# Methods of Estimation

---

- Holdout
  - Reserve 2/3 for training and 1/3 for testing
- Random subsampling
  - Repeated holdout
- Cross validation
  - Partition data into  $k$  disjoint subsets
  - $k$ -fold: train on  $k-1$  partitions, test on the remaining one
  - Leave-one-out:  $k=n$
- Stratified sampling
  - oversampling vs undersampling
- Bootstrap
  - Sampling with replacement

# Model Evaluation

---

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- **Methods for Model Comparison**
  - How to compare the relative performance among competing models?

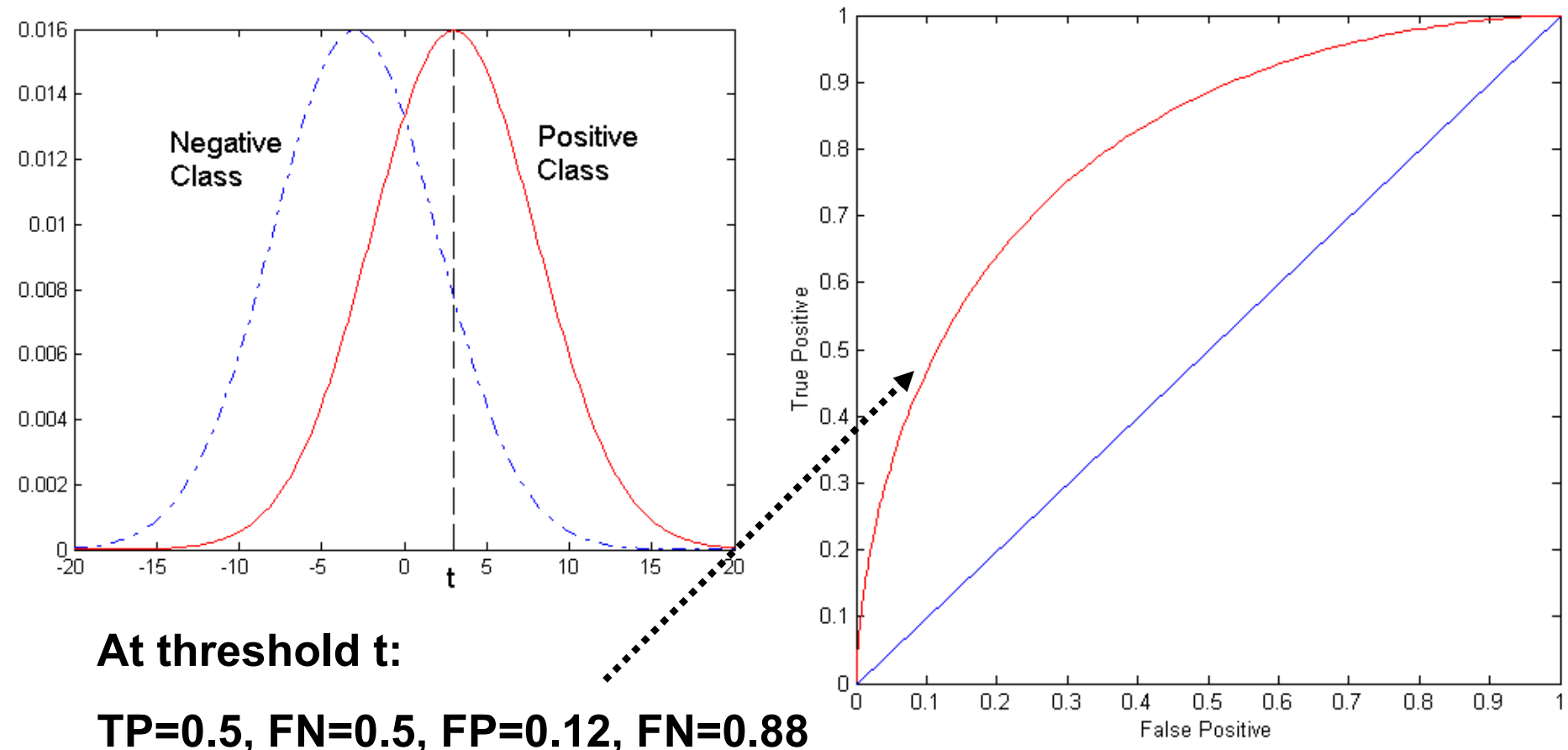
# ROC (Receiver Operating Characteristic)

---

- Developed in 1950s for signal detection theory to analyze noisy signals
  - Characterize the trade-off between positive hits and false alarms
- ROC curve plots TP (on the y-axis) against FP (on the x-axis)
- Performance of each classifier represented as a point on the ROC curve
  - changing the threshold of algorithm, sample distribution or cost matrix changes the location of the point

# ROC Curve

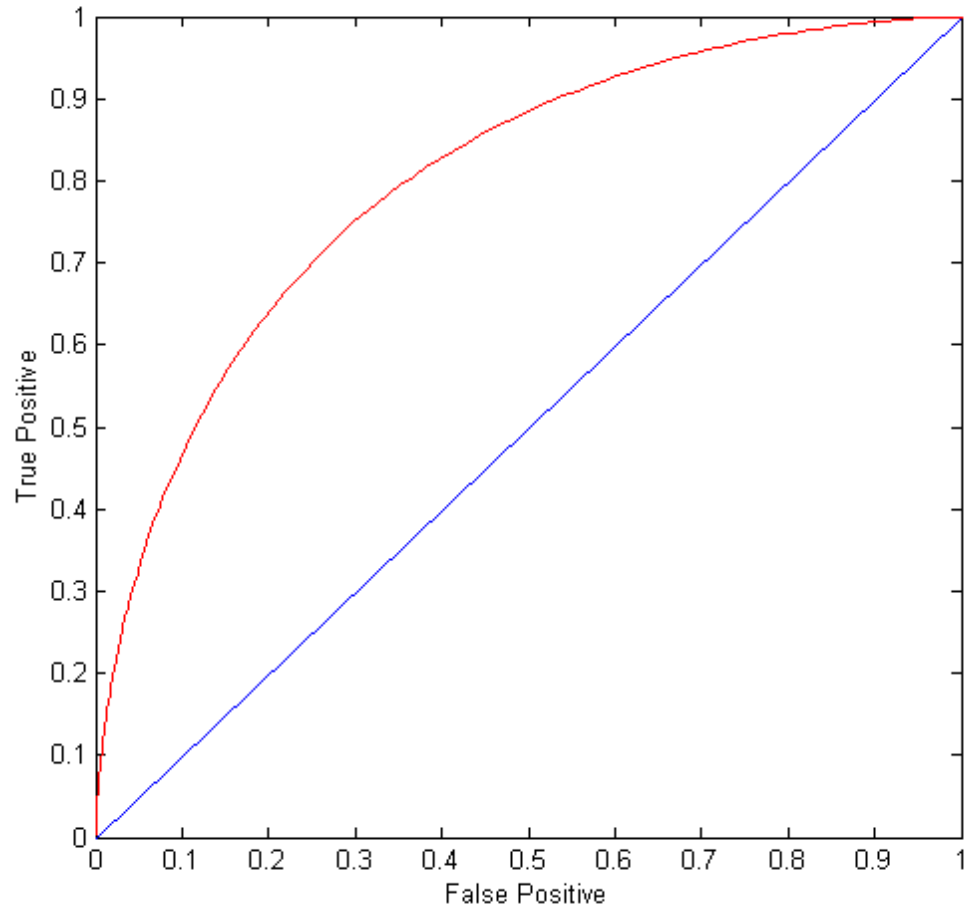
- 1-dimensional data set containing 2 classes (positive and negative)
- any points located at  $x > t$  is classified as positive



# ROC Curve

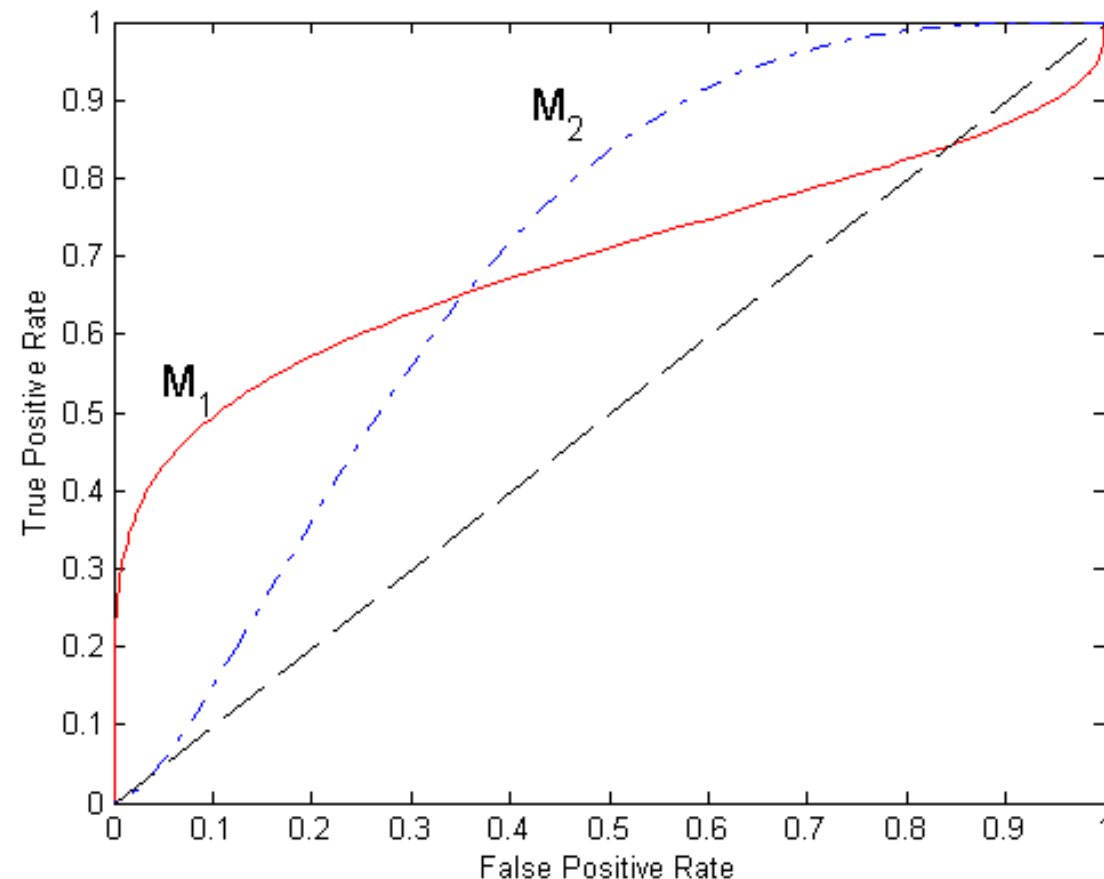
(TP,FP):

- (0,0): declare everything to be negative class
- (1,1): declare everything to be positive class
- (1,0): ideal
- Diagonal line:
  - Random guessing
  - Below diagonal line:
    - ◆ prediction is opposite of the true class





# Using ROC for Model Comparison



- No model consistently outperform the other
  - $M_1$  is better for small FPR
  - $M_2$  is better for large FPR
- Area Under the ROC curve
  - Ideal:
    - Area = 1
  - Random guess:
    - Area = 0.5

# How to Construct an ROC curve

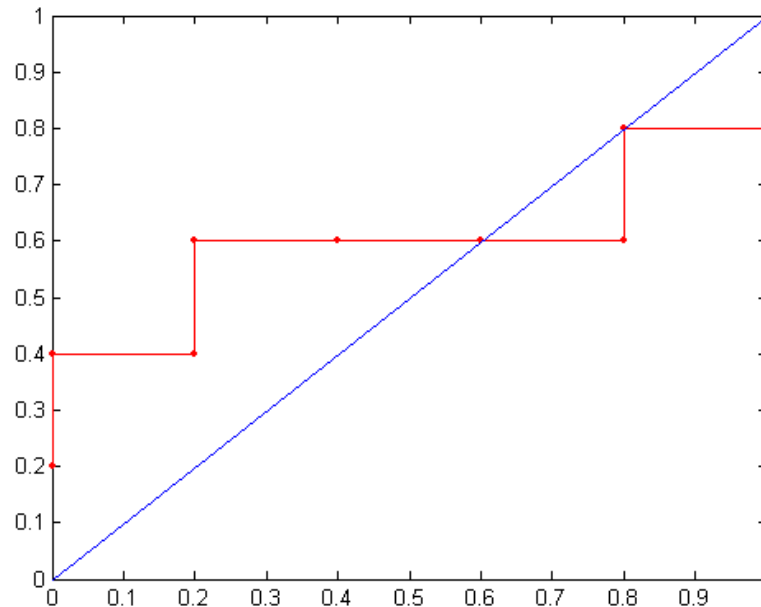
Instance	$P(+ A)$	True Class
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

- Use classifier that produces posterior probability for each test instance  $P(+|A)$
- Sort the instances according to  $P(+|A)$  in decreasing order
- Apply threshold at each unique value of  $P(+|A)$
- Count the number of TP, FP, TN, FN at each threshold
- TP rate,  $TPR = TP/(TP+FN)$
- FP rate,  $FPR = FP/(FP + TN)$

# How to construct an ROC curve

Class	+	-	+	-	-	-	+	-	+	+	
Threshold $\geq$	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3	3	3	2	2	1	0
FP	5	5	4	4	3	2	1	1	0	0	0
TN	0	0	1	1	2	3	4	4	5	5	5
FN	0	1	1	2	2	2	2	3	3	4	5
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4	0.2	0
FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0	0	0

ROC Curve:



# Test of Significance

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- Given two models:
  - Model M1: accuracy = 85%, tested on 30 instances
  - Model M2: accuracy = 75%, tested on 5000 instances
- Can we say M1 is better than M2?
  - How much confidence can we place on accuracy of M1 and M2?
  - Can the difference in performance measure be explained as a result of random fluctuations in the test set?

# Confidence Interval for Accuracy

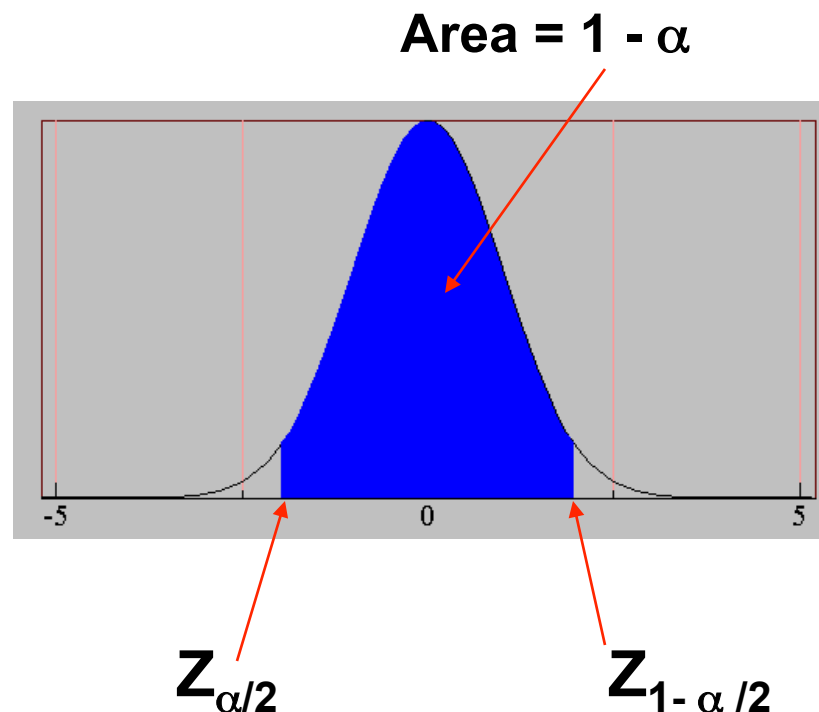
- Prediction can be regarded as a Bernoulli trial
  - A Bernoulli trial has 2 possible outcomes
  - Possible outcomes for prediction: correct or wrong
  - Collection of Bernoulli trials has a Binomial distribution:
    - ◆  $x \sim \text{Bin}(N, p)$       $x$ : number of correct predictions
    - ◆ e.g: Toss a fair coin 50 times, how many heads would turn up?  
Expected number of heads =  $N \times p = 50 \times 0.5 = 25$
- Given  $x$  (# of correct predictions) or equivalently,  $\text{acc} = x/N$ , and  $N$  (# of test instances),

Can we predict  $p$  (true accuracy of model)?

# Confidence Interval for Accuracy

- For large test sets ( $N > 30$ ),
  - acc has a normal distribution with mean  $p$  and variance  $p(1-p)/N$

$$P\left(Z_{\alpha/2} < \frac{acc - p}{\sqrt{p(1-p)/N}} < Z_{1-\alpha/2}\right) = 1 - \alpha$$



- Confidence Interval for  $p$ :

$$p = \frac{2 \times N \times acc + Z_{\alpha/2}^2 \pm \sqrt{Z_{\alpha/2}^2 + 4 \times N \times acc - 4 \times N \times acc^2}}{2(N + Z_{\alpha/2}^2)}$$

# Confidence Interval for Accuracy

- Consider a model that produces an accuracy of 80% when evaluated on 100 test instances:
  - $N=100$ ,  $\text{acc} = 0.8$
  - Let  $1-\alpha = 0.95$  (95% confidence)
  - From probability table,  $Z_{\alpha/2}=1.96$

N	50	100	500	1000	5000
p(lower)	0.670	0.711	0.763	0.774	0.789
p(upper)	0.888	0.866	0.833	0.824	0.811

$1-\alpha$	Z
0.99	2.58
0.98	2.33
0.95	1.96
0.90	1.65

# Comparing Performance of 2 Models

- Given two models, say M1 and M2, which is better?
  - M1 is tested on D1 (size= $n_1$ ), found error rate =  $e_1$
  - M2 is tested on D2 (size= $n_2$ ), found error rate =  $e_2$
  - Assume D1 and D2 are independent
  - If  $n_1$  and  $n_2$  are sufficiently large, then

$$e_1 \sim N(\mu_1, \sigma_1)$$

$$e_2 \sim N(\mu_2, \sigma_2)$$

- Approximate:  $\hat{\sigma}_i = \frac{e_i(1-e_i)}{n_i}$



# Comparing Performance of 2 Models

- To test if performance difference is statistically significant:  $d = e1 - e2$ 
  - $d \sim N(d_t, \sigma_t)$  where  $d_t$  is the true difference
  - Since D1 and D2 are independent, their variance adds up:

$$\begin{aligned}\sigma_t^2 &= \sigma_1^2 + \sigma_2^2 \cong \hat{\sigma}_1^2 + \hat{\sigma}_2^2 \\ &= \frac{e1(1-e1)}{n1} + \frac{e2(1-e2)}{n2}\end{aligned}$$

- At  $(1-\alpha)$  confidence level,  $d_t = d \pm Z_{\alpha/2} \hat{\sigma}_t$

# An Illustrative Example

- Given: M1:  $n_1 = 30$ ,  $e_1 = 0.15$   
M2:  $n_2 = 5000$ ,  $e_2 = 0.25$
- $d = |e_2 - e_1| = 0.1$  (2-sided test)

$$\hat{\sigma}_d = \frac{0.15(1-0.15)}{30} + \frac{0.25(1-0.25)}{5000} = 0.0043$$

- At 95% confidence level,  $Z_{\alpha/2} = 1.96$

$$d_t = 0.100 \pm 1.96 \times \sqrt{0.0043} = 0.100 \pm 0.128$$

=> Interval contains 0 => difference may not be statistically significant

# An Illustrative Example

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The following table shows the values of  $Z_{\alpha/2}$  at different confidence levels:

$1 - \alpha$	0.99	0.98	0.95	0.9	0.8	0.7	0.5
$Z_{\alpha/2}$	2.58	2.33	1.96	1.65	1.28	1.04	0.67

# Comparing Performance of 2 Algorithms

- Each learning algorithm may produce k models:
  - L1 may produce M11 , M12, ..., M1k
  - L2 may produce M21 , M22, ..., M2k
- If models are generated on the same test sets D1,D2, ..., Dk (e.g., via cross-validation)
  - For each set: compute  $d_j = e_{1j} - e_{2j}$
  - $d_j$  has mean  $d_t$  and variance  $\sigma_t$
  - Estimate:

$$\hat{\sigma}_t^2 = \frac{\sum_{j=1}^k (d_j - \bar{d})^2}{k(k-1)}$$

$$d_t = \bar{d} \pm t_{1-\alpha, k-1} \hat{\sigma}_t$$